Laser ablation condensation and phase transitions of dense TiO2 particles

Complete Parameter Estimation of Induction Machines by Time-varied Parameters

A theory to guide family caregivers of people who are at risk of suicide

Derivation of Equations for the Electromagnetic Interactions between Molecular Solutes
Effectively extend the lifespan of fistula of Dialysis patients

Reduce the fistula reconstruction process.

I-Shou University, Department of Biomedical Engineering and Veterans General Hospital in collaboration developing fistula blood flow sound capture device

Good news and blessing for the dialysis patients! I-Shou University, chairman of Biomedical Engineering department, Dr. Jia-Jung Wang host the research project “Using the sound of blood flow analysis of non-invasive method in determine the degree of fistula blockage in dialysis patients. This can give a more accurate quantitative indicators and a timely reminder of the dialysis patients for the necessary medical treatments. The device can effectively extend the fistulas life of dialysis patients and reduce the process of reconstruction of fistula and further enhance the quality of care for dialysis patients.

There are about 60,000 dialysis patients in Taiwan, the highest in population ratio in the world. As the increase in aging population, there are about 8,000 new dialysis patients annually, and long-term dialysis patients need to use the arteriovenous fistula or artificial fistula (arteriovenous graft) as the blood pipeline in performing hemodialysis, 3-4 hours each time and three times a week. However, hemodialysis fistula often cause the narrowing diameter of blood vessel and thrombosis that lead to dysfunction. There are only sporadic effective quantitative indicators that can pre-assess the narrowing of artery and thrombosis in non-invasive manner by detective the blood flow noise to determine its smoothness or fingers touch physical examination by the medical personnel for assessment of the degree of blood flow. Therefore, Dr. Jia-Jung Wang, chairman of the department of Biomedical Engineering, indicated that their research development is a non-invasive method in measuring the amplitude and frequency distribution of noisy sound of fistula blood flow, from which to extract the quantitative indicators to assess the degree of fistula and through this can early accurately detective and assess the degrees of stenosis. This can timely remind the dialysis patients to have fistula shaping surgery beforehand, thus can effectively extending the life of the dialysis fistula and reduce the pain in fistula reconstruction surgery for dialysis patients and their medical costs.
New President of I-Shou University Dr. Jei-Fu Shaw: hopes for I-Shou University in becoming a international university with characteristics and actively developing the pharmaceutical biotechnology fields.

Make up for the gap in education between North and the South

Chairman of the Board of United Group and founder of the I-Shou University Mr. Lin I-Shou indicated that after the few presidents hard working in building the research foundations, I-Shou University has gradually becoming a comprehensive university. In 2000 I-Shou University first set up medical school in coping with the future of Taiwan's industry trends and development in health and bio technology fields. The development of the biotechnology industry is wishing to compensate the research and education resources gap between the north and the southern part of Taiwan. He recently appointed Dr. Jei-Fu Shaw as the new president of I-Shou University, in hoping to rely on President Jei-Fu Shaw’ professional specialties in biotechnology field and his wide contacts and personal academic connections to expand the biotechnology field in southern Taiwan, He specially wants to thank the leadership of substitute president Dr. Wan-Long Hong who give stability in both academic and school administration and services.

The New president Dr. Jei-Fu Shaw mentioned in his speech that because of the efforts and hard work of previous presidents, I-Shou University has been recognized by the Ministry of Education as a teaching with Excellence University. Under the existing solid foundations, he will use the past experiences he had when he was at Academia Sinica and as the president of National Chung Hsing University in upgrading Chung Hsing university into a top research university that is on the list of five-year 150 billion research universities support by the Ministry of Education. In the future, I-Shou University will upgrade into a both teaching excellence and outstanding research university among private universities that able to implement the outstanding achievements in innovation and industrial development.

Running objectives for the school: first, looking forward in making I-Shou University into a green Silicon Valley university and leading it in becoming a non-polluting and high-tech research
and development university. This should combined humanities, and technology in promoting the
development of culture and technology industry in southern Taiwan and emulate University of
Stanford that give birth to high-tech industries Silicon Valley in spurring California and world
development.

Second, cultivate the young talented elite to have international perspectives, innovative thinking
that have positively influence on society and country. The talented personnel must equipped with
innovative thinking, modern knowledge, health oriented, resistance to stress, communication skills
and attention to the society and country. This is done through courses teaching, community activities
and counseling that cultivate young talented personnel in making this school in becoming the country's
top-class University.

in addition, Enhance the development of concentration fields in making I-Shou university into a
university with academic characteristics that make into the world's top 100 university. third, Strengthen
the link of students' future employment with the Institutes and graduate schools; Fourth, strengthen
the research and development of teachers and patent and patent technology transfer, development of
innovative science and technology park, such as health biotech park which combined with the school’s
medical group Da Hospital; Finally, I-Shou University for continuing to draw on the successful
experience with industry, government, academic and research community, will establish”The
Advisory Committee of the school”, that adopt views from all parties, led I-Shou University into a
unique world-class university.
Only one among private universities! The Shining Star of Taiwan! I-Shou University department of nutrition and minister of E-Da hospital, professor Gin-Ho Lo Received the outstanding research prize from the National Science Council.

I-Shou University department of nutrition and minister of E-Da hospital, professor Gin-Ho Lo was awarded the Outstanding in research prize from the National Science Council. I-Shou was the only private university in Taiwan to received such an honor.

Chronic hepatitis B and hepatitis C patients are common in Taiwan, many patients often lead to cirrhosis of the liver disease are because of ineffective treatment that lead to merge in esophageal venous aneurysm bleeding or acute hemorrhage. the mortality rates is as high as 35%. It is due to the progress in medical technology that enables to reduce the mortality rate to 15 percent. Professor Gin-Ho Lo, from the department of nutrition, is the expertise in this area of study to prevent venous aneurysm bleeding through explore in clinical research and related cases investigation. This will effectively provide Taiwan cirrhosis patients in reducing mortality rates.

Professor Gin-Ho Lo of I-Shou University, department of nutrition, indicated that he thanks the National Science’s recognition again. The clinical research can received such an outstanding research award is certainly rare. through the I-Shou University and Da Hospital resource alliance effectively to create a medical research win-win situation, so that justice Shou University large hospitals and justice in the international light. Currently, he is actively seeking cooperation with the south of the major teaching hospitals and regional hospitals to increase the clinical case study, and joint R & D to reduce patient mortality and help prevent disease treatment, hope to benefit more patients.
Three Stars Received by I-Shou University in Selection Appraisal of International Resources by the Cheers

According to the latest issue of Cheers magazine in 2012 on the 100 academic year 65 universities in general international resource appraisal, I-Shou University received first place in three categories, “mainland exchange students”, “exchange students study in China” and “cross-border double degree” in private universities.

Cheers magazine published the 2012 assessment in general international resources in universities. The selection of indicators including public and private universities in “foreign degree students”, "foreign exchange students”, “undergraduate exchange students study abroad accounted for the percentage proportion of total undergraduate," the mainland exchange students” “students study in mainland”"and" cross-border double-degree number ",total of six categories. The survey of the magazine pointed out that I-Shou University in 100 academic years has number up to 463 exchange students from China. “The number of students study abroad in China has 53 people; and the “cross-border double degrees” is also up to 12 in numbers. This shows the positive efforts of I-Shou University in educational exchanges.

I-Shou University currently established 68 two-way exchange students partner schools with China of which 21 schools were among the 985 development emphasis plans, 37 schools in 211 plans. In addition, in the 101 academic year further emphasis on development of double degree cooperation and promoting double Degree Program with the development emphasis schools and other internationally renowned universities, so that future students of I-Shou university can study and keep pace with the China and international standards.
I-Shou University Departments in Engineering 29 school system Awarded the IEET certificates.

Fully Aligned with international education

The teaching and research performances by I-Shou University has received international certification recognitions. Nine department and 29 school systems were awarded the Engineering and Technology education certificates in 100 academic year by the Institute of Engineering Education Taiwan.

According to the IEET100 academic year certification results indicated that all the departments from the college of electrical engineering and information engineering and college of science and engineering, department of civil and ecological engineering, department of chemical engineering, department of biomedical engineering, department of materials science and engineering, department of communication engineering, department of information engineering, department of electrical engineering, department of mechanical and automation engineering, total of 9 departments from the undergraduate, master to doctoral programs of 29 school system were awarded the IEET engineering and technology certifications. The results shown the teaching and academic quality of I-Shou University had reached the international professional recognitions. While other universities, colleges, technical colleges faced with the educational evaluation by the ministry of Education. The IEET certification has make I-Shou university free from by the Ministry of Education.

The president of I-Shou University, Dr. Jei-Fu Shaw emphasized that the 9 departments, civil, chemical, biomedical, materials, communications, and Information Engineering, Electronic, Electrical, Mechanical all passed the "IEET certifications which represent the school in teaching and research quality in information and engineering and students’ learning capacity has reached international standards. The students after graduation can use the I-Shou University degrees connecting to the multi-country of the world and obtain a professional engineer licenses. Finally, the job market is no longer confined to only Taiwan and can more fully aligned with international companies.
Abstract

High-pressure phase of TiO$_2$ with $\alpha$-PbO$_2$-type and baddeleyite-type related structure has been synthesized via very energetic Nd-YAG laser pulse irradiation of oxygen-purged Ti target. The nanometer-size $\alpha$-PbO$_2$-type particles were (110), (010) and (001) faceted but the larger ones were spherical. Spherical nanoparticles of fluorite structure transformed martensitically into baddeleyite-type and then $\alpha$-PbO$_2$-type structures with accompanied transformation twinning, shearing and shape change into ellipsoid upon electron irradiation. The relatively large particles followed the same transformation path yet with alternative lattice correspondence and additional multiple deformation twinning of the baddeleyite type. The combined effects of rapid heating and cooling, the nanosize effect and dense surfaces account for the formation of the dense TiO$_2$ polymorphs particles.

Keywords: laser ablation, TiO$_2$, fluorite, high-pressure phase

Introduction

Dense TiO$_2$ polymorphs, i.e. post-rutile (isostructure with stishovite SiO$_2$) phases, of acknowledged response to static and dynamic high pressure may reveal fundamental information about the behavior of analogue oxides in crustal rocks attending subduction into Earth’s interior and natural dynamic events. These
dense polymorphs include: $\alpha$-PbO$_2$-type (Figure 1, space group Pbcn); baddeleyite-type (MI, fluorite-related type P2\textsubscript{1}/c) (presumably fluorite or distorted fluorite structure, Figure 2); OI (Pbca); and cotunnite (PbCl$_2$-type, i.e. OII, Pnma) in the order of increasing density\textsuperscript{[1,2]}. Recently, an $\alpha$-PbO$_2$-type TiO$_2$ has been reported to occur as a nanometer slab in a rutile twin bicrystal inclusion in garnet from diamondiferous quartzofeldspathic rocks from the Saxonian Erzgebirge indicating a burial of continental crustal rocks to depths of at least 130 kilometers\textsuperscript{[3]}. On the other hand both $\alpha$-PbO$_2$-structured and baddeleyite-structured polymorphs were found in shocked gneisses from the Ries crater in Germany indicating peak shock pressure\textsuperscript{[4,5]}. The results of large-scale molecular dynamics simulations demonstrate that the mechanisms responsible for material ejection as well as most of the parameters of the ejection process have a strong dependence on the rate of the laser energy deposition\textsuperscript{[6-9]}. For longer laser pulses, in the regime of thermal confinement, a phase explosion of the overheated material is responsible for the collective material ejection at laser fluences above the ablation threshold. This phase explosion leads to a homogeneous decomposition of the expanding plume into a mixture of liquid droplets and gas phase molecules. The decomposition proceeds through the formation of a transient structure of interconnected liquid clusters and individual molecules and leads to the fast cooling of the ejected plume. For shorter laser pulses, in the regime of stress confinement, a lower threshold fluence for the onset of ablation is observed and attributed to photomechanical effects driven by the relaxation of the laser-induced pressure. Larger and more numerous clusters with higher ejection velocities are produced in the regime of stress confinement as compared to the regime of thermal confinement. For monomer molecules, the ejection in the stress confinement regime results in broader velocity distributions in the direction normal to the irradiated surface, higher maximum velocities, and stronger forward peaking of the angular distributions. The acoustic waves propagating from the absorption region are much stronger in the regime of stress confinement and the wave profiles can be related to the ejection mechanisms. Based on Fabbro
and co-workers’ studies\[10\], a shock wave induced by the laser-induced plasma (LIP) is created in the plasma plume due to the confinement of environment. The laser-induced plasma adiabatically expands at a supersonic velocity to create a shock wave under confinement, when it absorbs the later part of the laser pulse and gets a continual supply of the vaporizing species from the solid target. Then, the shock wave will induce an extra pressure in the laser-induced plasma. The pressure increase induced by the shock wave to be the plasma-induced pressure. Further, the plasma-induced pressure will lead to an additional temperature increase of the laser-induced plasma. Therefore, the shock wave generated by the expansion of the laser-induced plasma under confinement pushes the laser-induced plasma into a thermodynamic state of the higher temperature, higher pressure and higher density than that of the initially generated plasma by creating the additional pressure and temperature increases in the laser-induced plasma. Accordingly, uniquely produced laser-induced plasma of high temperature, high pressure and high density, is generated when the laser pulse irradiated the surface of the solid target. Since the laser-induced high-density plasma is in the state with high temperature and high pressure, the new phase, especially the metastable phase, could form by the high-temperature chemical reactions between the ablations from the target. Note that the thermodynamic state with high temperature, high pressure, and high density is obviously favorable for the formation of the metastable phases that are in the high-temperature and high-pressure region on their thermodynamic equilibrium phase diagram.

Here we report the first successful laser-ablation condensation of α-PbO₂-type TiO₂ as well as particle supporting spectroscopic evidence for a condensation of dense oxides around presolar stars. Besides, we also analysis baddeleyite-type related TiO₂ nanoparticles which remained unchanged upon quenching to ambient pressure, but transformed spontaneously into a baddeleyite-type structure upon electron irradiation. We emphasize the size-dependent shape change due to surface vs. coherency strain energetics and cell volume change as a result of residual stress level, which are important in view of the current discussion of the high-pressure behavior of nanosized oxide particles.

**Experimental**

We used Nd-YAG-laser (JK laser, 1.06 m in wavelength, beam mode: TEM00) pulse irradiation at a specific pulse time duration (2.4 ms at 30 Hz), spot size (0.146 mm²), optimal energy input (0.5 to 2 J/pulse) and oxygen flow (20 L/min) along the laser beam direction to vaporize the Ti target inside an ablation chamber under 1 atm for the synthesis of the TiO₂ condensates. Titania crystallites formed under such conditions are typically 5 nm to 60 nm in size and are predominantly anatase, with minor rutile, α-PbO₂ type\[1,2\] as well as extra baddeleyite-type related TiO₂ that is the focus of this study. The condensates produced at 0.5 J/pulse and an oxygen flow rate of 20 L/min were used for the present study of the phase change
Identification of TiO$_2$ dense structure

Titania crystallites formed under optimum condition of laser ablation condensation are typically 5 nm to 60 nm in size (Fig. 3). SAED from an area of about 0.8 $\mu$m$^2$ indicated that these randomly oriented TiO$_2$ particles are predominantly anatase, with minor rutile and other structure (not shown). Scrutiny of the three ring-diffractions not superimposed with those of anatase and rutile indicated that they fit (111), (020) and (220) diffractions of $\alpha$-PbO$_2$-type TiO$_2$. Lattice image and two-dimensional Fourier transforms of the images (not shown) indeed identified nanometer-size (e.g. 8, 10 and 25 nm) $\alpha$-PbO$_2$-type TiO$_2$ particles (arrowed in Fig. 3) all with an interfacial angle of 81 degree for (1 $\bar{1}$ 0) and (110) faces and preferentially [001]-oriented due to a habit plane of (001)[1]. A high-pressure polymorph can be stabilized via nanometer-size effect, in terms of surface energy minimization. The surface energy of $\alpha$-PbO$_2$-type TiO$_2$ is lower than that of the rutile according to a depression of the phase transition pressure due to nanophase effect for the V-shaped equilibrium pressure-temperature (P-T) phase boundary of $\alpha$-PbO$_2$-type TiO$_2$/rutile.$^1$. The radiant cooling rate, after the pulse was extinguished, was estimated to be $1 \times 10^9$ K/s for 10 nm particle using an expression pertinent to laser pulses and background gas effect and assuming that the density and heat capacity of the molten state are similar to those of its solid-state counterpart rutile with a common radiant emissivity of transition metal oxides. This cooling rate is about 3 orders of magnitude higher than the threshold ($1.6 \times 10^6$ K/s) for metastable phase formation in pulsed laser deposition process. Residual stress as a result of a high cooling rate was known to preserve metastable quenched states of condensed phases. Given the refined cell parameters $a = 0.461$ nm, $b = 0.543$ nm, $c = 0.487$ nm and reported parameters of the Birch-Murnaghan equation of state, i.e. $K_T = 258(8)$ GPa, $K' = 4.05(25)$, and $\rho_o = 4.336(12)$ g/cm$^3$ for synthetic $\alpha$-PbO$_2$-type TiO$_2$, we obtained a molar volume of 18.35 cm$^3$/mol for the large spherical $\alpha$-PbO$_2$-type TiO$_2$ particle in Figure 3. This could indicate that the particles formed by condensation have a residual stress of about 0.96 GPa, which could somehow help stabilize the $\alpha$-PbO$_2$-type structure. The fact that the $\{110\}$ d-spacing decreases with decreasing size indicates
an even higher residual stress for nanoparticles. Assuming isotropic compression, a \{110\} d-spacing of 0.346 nm gives a molar volume of 18.21 cm$^3$/mol, and a residual stress of 3 GPa for the 8 nanometer-size particle. Given this residual stress level, the nanometer-size \(\alpha\)-PbO$_2$-type TiO$_2$ particles were fairly retained for more than a year at room P-T condition.

The baddeleyite-type related particles are too small in content to produce diffraction rings, but can be identified individually by lattice image and single-crystal diffraction pattern. Figure 4(a) shows typically a condensed TiO$_2$ particle partially transformed upon electron irradiation into baddeleyite type in the [001] zone axis with lattice planes indexed according to a distorted version of a cubic fluorite cell as adopted for zirconia$^{[2]}$. The two-dimensional Fourier transform from the square region in Fig. 4(a) shows that diffraction spots definitely belong to the baddeleyite type and weaker spots are attributable to fluorite-like TiO$_2$ with slight distortion. Schematic indexing of the diffraction pattern shows that the fluorite-like (denoted as f-) and monoclinic baddeleyite-type (denoted as m-) TiO$_2$ have a specific crystallographic relationship, i.e., [001]$_f$/[001]$_m$; (010)$_f$/([1 0 1 0])$_m$, or alternatively (1 1 0)$_f$/(1 0 0)$_m$ for a twin variant of m-phase. The diffraction spots of the relic fluorite-like TiO$_2$ are not strong because they are contributed only from area I in the reconstructed image. This sheds light on a fluorite-like parent structure in three dimensions in accordance with a structure denser than its derivative associated with relaxation, i.e., the baddeleyite-type. The baddeleyite-type TiO$_2$ shows twinned domains with (110) twin plane and (001) twin axis as indicated by the magnified region II twin axis with inset schematic drawing. While obtaining the diffraction pattern under a 25 nm beam size, this particle transformed completely into an \(\alpha\)-PbO$_2$ type full of edge dislocations with (1 1 0) and (100) slip planes (Fig. 4b)$^{[2]}$. The refined monoclinic cell parameters are $a = 0.465 \pm 0.003$ nm, $b = 0.493 \pm 0.002$ nm, $c = 0.496 \pm 0.004$ nm, and $\beta = 99.31 \pm 1.60^\circ$, in close agreement with those of natural materials from the Ries crater. Given the refined cell parameters and reported parameters of the Birch-Murnaghan equation of state, i.e., isothermal bulk modulus $K_T = 304$ GPa, $K' = 3.9$ and zero-pressure molar volume $V_0 = 16.90$ cm$^3$/mol, a residual stress of 1.1 GPa was then calculated for baddeleyite-type TiO$_2$. As for the parent relic possibly with a fluorite-like structure, it has no sufficient and reliable data for the estimation of residual stress$^{[2]}$. 

![Figure 3](image.png)

**Figure (3)** TEM lattice images of \(\alpha\)-PbO$_2$ type TiO$_2$, scale bare equal to 5 nm.
The relatively large fluorite-type particles also transformed upon electron irradiation into baddeleyite type (Fig. 5a) and then partially into α-PbO$_2$ type Fig. 5(b) yet with a lattice correspondence $[010]_m//[100]_a$; $(100)_m//(02\overline{1})_a$ different from that of nanosized particles, and are complicated by primary and secondary deformation twin variants of the baddeleyite type following {100} and {110} twin planes$^{[2]}$. The transverse twinning substructure is analogous to that within monoclinic particles of partially stabilized zirconia to accommodate strain. Extensive shape change accompanied with phase transformations and deformation always caused a focusing problem for these large particles.

In the following, possible transformation schemes of baddeleyite-type related polymorphs of TiO$_2$ are proposed in terms of topological distortions of three-dimensional anion nets for dioxides$^{[2]}$. As depicted schematically in Fig. 6, every other (010) anion plane of ideal fluorite-type TiO$_2$ viewed edge-on in [001] projection Fig. 6(a) shears along opposite [100], directions to form twinned baddeleyite type with 7-coordinated rhomb rows Fig. 6(b). Further homogeneous
shear along [100], accounts for the formation of \( \alpha\)-PbO\(_2\)-type with zigzag triangular rows, i.e., edge-sharing 6-coordinated octahedral chains, running along the [001] direction Fig. 6(c). The relationship \((100)_{m}//(02 \overline{1})_{a}\) for relatively large particles (Fig. 5) implies alternative [010] shuffling possibly to accommodate strain. In this case, a rather homogeneous shear across m-twin variants may be required to generate edge-sharing octahedral chains of the \( \alpha\)-PbO\(_2\)-type structure Fig. 6(d). The T-P phase boundaries of baddeleyite/\( \alpha\)-PbO\(_2\)-type TiO\(_2\) and \( \alpha\)-PbO\(_2\)-type TiO\(_2\)/Rutile were determined by static compression coupled with various heating techniques (Fig. 6e). At a higher T-P, the OI structure and cotunnite type with seven- and nine-coordinated cations, respectively, were synthesized by static compression coupled with laser heating under conditions shown in Fig. 6(e).

Figure (6) transformation schemes of baddeleyite-type related polymorphs of TiO\(_2\)
Conclusions

We focused on the synthesis of laser-ablation condensation of α-PbO$_2$-type TiO$_2$ particle as well as size-dependent phase and shape changes of the baddeleyite-type related particles upon electron irradiation, which are important in view of the relaxation path of dense TiO$_2$ and the current discussion of the martensitic transformation of nanosized particles free of matrix constraint. The nanometer-size α-PbO$_2$-type particles were (110), (010) and (001) faceted but the larger ones were spherical. Spherical nanoparticles of fluorite structure transformed martensitically into baddeleyite-type and then α-PbO$_2$-type structures with accompanied transformation twinning, shearing and shape change into ellipsoid upon electron irradiation. The relatively large particles followed the same transformation path yet with alternative lattice correspondence and additional multiple deformation twinning of the baddeleyite type. The combined effects of rapid heating and cooling, the nanosize effect and dense surfaces account for the formation of the dense TiO$_2$ polymorphs particles.

References

Complete Parameter Estimation of Induction Machines by Time-varied Parameters

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Abstract

This paper uses time-varied signals of voltage, current and rotor speed to compute the equivalent circuit parameters, moment of inertia, and friction coefficient of an induction machine. A time-varied impedance can be found by the time-varied voltage and current. From the variation of impedance to the rotor speed, the parameters of equivalent circuit can be found. According to the equivalent circuit and rotor speed, the torque can be found via established dynamic system model. On the basis of torque and rotor speed with time, moment of inertia and friction coefficient of the motor can be obtained. This paper uses the gradient method to solve the above parameters. The initial values of least mean square are also described in this paper. This paper used estimated parameters to simulate the starting states of an induction machine to compare with the real one, accordingly, practicability and accuracy of this method has been proven.

Key words: Time-varied impedance, equivalent circuit, induction motor, gradient method.

Introduction

The stator of a three-phase induction machine has three-phase windings. The field doesn’t require the dc current when the rotor is running. By the relative motion of the rotor to the 1
stator magnetic field, the rotor induces voltage and current, furthermore, the torque causes the field interaction of rotor and stator. Owing to their simplicity and ease of operation, induction motors have become the most popular electric machine and are the most important one used in industry applications.

To establish an equivalent model of induction machines is very important for predicting machine performance and designing control schemes [1]. Over the past few decades, these research studies can be divided into online and offline identification systems [2,3]. In offline identification, the relative parameters of an induction machine can be found by standard tests, including the locked rotor test, the no-load test, and the stand-still frequency response test [4]. In online identification, the spectrum method can estimate parameters via the features of the system [5,6]. The model reference adaptive systems use the error between estimated and referenced measurements to calculate the parameters [7,8]. The artificial intelligence method uses the artificial neural network model instead of the model reference adaptive system. [9,10]. The additional signal was also injected in induction machines to establish the saturated model.

It is an extremely complex task to analyze accurate parameters of induction machines. The variation of resistance is about 1.2 times between normal atmospheric and rating temperatures. The reactances may change 1.4 times from saturated to unsaturated [11]. Core loss, rotating loss, and stray loss are about 5-10% of the full load [12]. An obvious striction exists in the rotating performance, which causes an equation of rotation that is difficult to solve. The consideration of the deep bars effect will complicate the model [13]. Furthermore, the above slight variations are usually concealed in the noise and quantization errors. However, it is worth improving the accuracy of the result, to obtain the complete parameters and simplify the complexity of testing.

This paper proposes a method to estimate the complete parameters of the induction machine by starting stage test, which significantly simplifies and saves cost for induction machine tests. Owing to the method for analyzing time-varied parameters, the parameter variation of the induction machine can be found within several milliseconds but not only from the effective values [14]. It makes the analysis for rapidly varying parameters of small-scale induction machines efficient. This method uses the voltage, current and rotor speed under this stage to estimate such relative parameters. The equivalent circuit of the machine is determined by the variation of impedance versus rotor speed. By the parameter of equivalent circuit and rotor speed, the user can simulate the dynamic performance of the induction machine. This paper calculates the output torque by dynamic simulation, and furthermore, the moment of inertia and friction coefficient will be found via the data of output torque and rotor speed. This paper uses the least mean square (LMS) method to obtain the parameters which can conform to the practical performance. The optimal solution searching of the LMS is accomplished by the gradient method,
which is a series of iterations matching the set values to the real ones as far as possible. As a set of suitable initial values will help in enhancing the efficiency and convergence of iteration, this paper also proposes a way to set such values.

**Theory**

A. Impedance under Different Slip Rate

Models of induction machines can be divided into steady and transient models. In the primary state of starting, since the time constant is short enough, the transient state of the circuit will decay to a range that can be ignored, while steady impedance holds variance of voltage and current. The steady state equivalent circuit is shown in Fig. 1. Where $R_s$ is the stator resistance, $R_r$ is the rotor resistance, $X_s$ is the stator reactance, $X_r$ is the rotor reactance, $X_m$ is the magnetizing reactance, and $s$ is the slip rate. In Fig.1, the resistance and reactance on the primary side are given by

$$R(s) = R_s + \frac{X^2}{s} \frac{R_r}{(R_r/s)^2 + (X_m + X_s)^2}$$

$$X(s) = X_s + X_m - \frac{X^2(X_m + X_r)}{(R_r/s)^2 + (X_m + X_r)^2}$$

In Fig.1, only $R_r/s$ is affected by the slip rate and becomes a time-varied resistance. The variation influences the resistance and the reactance of the primary side, which become time-varied impedances. When the rotor speed varies from static state to the synchronous speed, the slip rate ranges from 0 to 1, and variations of resistance and reactance are shown in Fig.2.

In Fig.2, curve of the reactance is decreasing. The value is smooth within the primary stage of starting. And in the primary stage of starting, the resistance varies linearly. When rotor speed is close to synchronicity, a maximum value occurs. The values of resistance and reactance also intersect within this range. When the rotor speed continuously increases, the resistance rapidly decreases, and under the condition of the slip rate being equal to zero, the resistance is close to zero.

B. Gradient Method

The user will meet three problems in determining parameters of induction machines. Firstly, because the primary and secondary leakage reactances are far smaller than the magnetization reactance, the relationship of these two reactances is closely dependent. Secondly, the practical signal will be disturbed with noise, and these disturbances will create results. Finally, the practical system is more complex than the
considered model, and will make result error. To overcome these problems, this paper uses the gradient method to obtain the parameters which can conform to the practical performance.

The gradient method, also known as steepest descent method, may obtain the minimum value of the several variable nonlinear functions and find the optimal solution of the function. Its cardinal principle is taking gradients as derivatives of objective functions as the searching direction, and using the gradient method to solve parameters of the induction machine, the objective functions can be set as

\[
E_R = \sum_{i=0}^{14} \left[ R(s) - R_s - \frac{X_s^2 R_r / s \left( (X_r / s)^2 + (X_m + X_r)^2 \right)}{(R_r / s)^2 + (X_m + X_r)^2} \right]^2
\]

(3)

\[
E_X = \sum_{i=0}^{14} \left[ X(s) - X_s - X_m + \frac{X_s^2 (X_m + X_r)}{R_r / s + (X_m + X_r)^2} \right]^2
\]

(4)

\[
R_{\pm} = R_s - \eta_{X_s} \left( \frac{\partial E_R}{\partial R_s} \right) \]

(15)

\[
R_{\pm} = R_s - \eta_{X_s} \left( \frac{\partial E_X}{\partial R_s} \right) \]

(16)

\[
X_{\pm} = X_s + \eta_{X_s} \left( \frac{\partial E_R}{\partial X_s} \right) \]

(17)

\[
X_{\pm} = X_s + \eta_{X_s} \left( \frac{\partial E_X}{\partial X_s} \right) \]

(18)

\[
X_{\pm} = X_s - \eta_{X_s} \left( \frac{\partial E_X}{\partial X_m} \right) \]

(19)

where \( \eta_{X_s}, \eta_{R_s}, \eta_{X_s}, \eta_{X_r}, \) and \( \eta_{X_m} \) are known as
acceleration factors. The objective functions can be reduced by modifying parameters based on (15) to (19).

C. Initial Value Setting

Suitable initial values could promote the effect of convergence. This paper uses a set of equations to compute the approximate parameters of an induction machine. For distinctive representation, the symbols are illustrated in Fig. 3, which is the slip-impedance characteristic curve. The rotor speed normally cannot reach synchronicity. This paper proposes a set of initial values under this practical condition. In the slip rate \( s = 1 \), \( R(1) \) and \( X(1) \) can be found. In the slip rate \( s = 0.5 \), \( R(0.5) \) can be found. When the rotor speed is near synchronicity, two slip rates \( s_1 \) and \( s_2 \), which are near to zero, are obtained. Corresponding to these two slip rates, reactance \( X(s_1) \) and \( X(s_2) \) can be found. And then initial values of parameters can be calculated by the following way.

\[
R(s) \cong R_y + R_r / s, \quad 0.5 < s < 1
\]

Hence, the initial value of the resistance is

\[
R_y = 0.5(R(0.5) - R(1))
\]

and

\[
R_r = R(1) - R_y
\]

During the primary stage of starting, the reactance variance is very small and is approximately the sum of \( X_s \) and \( X_r \). This paper assumes initial value of the rotor reactance is equal to that of the stator reactance, so

\[
X_s = X_r = 0.5X(1)
\]

The magnetizing reactance can be found at no-load speed. When the rotor speed accelerates to the synchronized condition, the reactance is \( X(0) = X_s + X_m \). In the practical measurement, reaching this state will require more complex equipment. This paper used the extrapolation method, where accurate results could be also obtained using more simple equipment. When the rotor speed is approximately synchronous, the reactance increases linearly, and hence the reactance can be computed by the state approaching synchronicity. Based on the extrapolation method, the magnetizing reactance at synchronicity can be found as

\[
X_m = X(s_1) + \frac{s_1}{s_2 - s_1}(X(s_1) - X(s_2)) - X_s
\]

D. Dynamic Simulation

By mathematics, the user can establish a steady and dynamic model, and analyze the operated performance. This paper uses dynamic simulation to calculate the torque. The parameters of equivalent circuit have been found by the above-mentioned method, and the dynamic model of a 3-phase induction machine can be described.
in stator reference frames as

\[ v_{qs} = (R_s + L_s p)i_{qs} + L_m p_i_{qr} \]  \hspace{1cm} (25) \\
\[ v_{ds} = (R_s + L_s p)i_{ds} + L_m p_i_{dq} \]  \hspace{1cm} (26) \\
\[ v_{qr} = L_m i_{qs} - \omega L_i_{ds} + (R_s + L_s p)i_{qr} - \omega L_i_{dr} \]  \hspace{1cm} (27) \\
\[ v_{dr} = \omega L_i_{qr} + L_m i_{ds} + \omega L_i_{iq} + (R_s + L_s p)i_{dr} \]  \hspace{1cm} (28)

Where \( i_{q_s}, i_{d_s} \) are stator currents, \( i_{q_r}, i_{d_r} \) are rotor currents, \( v_{q_s}, v_{d_s} \) are stator voltages, \( v_{q_r}, v_{d_r} \) are rotor voltages, \( \omega \) is rotor speed, and \( P \) is the differentiation operator. Therefore, the output torque could be obtained:

\[ T = 3PL_m(i_{dr}i_{q_s} - i_{q_r}i_{ds}) \]  \hspace{1cm} (29)

where \( P \) is the number of poles.

Assuming that the torque is only for rotor speed but not for the load, the electromechanical dynamic equation is given by

\[ J\dot{\omega}_r + B\omega = T \]  \hspace{1cm} (30)

where \( J \) and \( B \) are the moment of inertia and the friction coefficient individually.

D. Moment of Inertia and Friction Coefficient

The moment of inertia and friction coefficient can determine the relationship between torque and rotor speed. That is, if torque and rotor speed are known, the moment of inertia and friction coefficient can be found. The relationship in sequence data can be written as

\[ J(\omega_r(n) - \omega_r(n-1)) + B\omega_r(n) = T(n) \] , \( n = 0,1,\ldots \)  \hspace{1cm} (31)

Consider the system is linear, then this moment of inertia and friction coefficient is constant, and the suitable parameters can be set by objective function.

\[ E_r = \frac{1}{N-1} \sum_{n=1}^{N-1} \left( T(n) - J(\omega_r(n) - \omega_r(n-1)) - B\omega_r(n) \right)^2 \]  \hspace{1cm} (32)

The optimal solutions of \( J \) and \( B \) are obtained in the case of the objective function being a minimum, that is, under the condition of both gradients of (32) to \( J \) and \( B \) being equal to zero. Therefore, \( J \) and \( B \) can be found as

\[ \begin{bmatrix} J \\ B \end{bmatrix} = \begin{bmatrix} \sum_{n=0}^{N-1} (\omega_r(n) - \omega_r(n-1)) & \sum_{n=0}^{N-1} (\omega_r(n) - \omega_r(n-1))^2 \\ \sum_{n=0}^{N-1} (\omega_r(n) - \omega_r(n-1))^2 & \sum_{n=0}^{N-1} (\omega_r(n))^2 \\ \sum_{n=0}^{N-1} T(n)(\omega_r(n) - \omega_r(n-1)) & \sum_{n=0}^{N-1} T(n)\omega_r(n) \\ \sum_{n=0}^{N-1} T(n)\omega_r(n) & \sum_{n=0}^{N-1} T(n) \\ \end{bmatrix} \]  \hspace{1cm} (33)

F. Procedure

This section arranges the above-mentioned theory as a complete procedure.

Step 1: Time-varied parameters: The voltage, current, and rotor speed at starting state of an induction machine are given.

Step 2: Impedance in different slip rates: The resistance and reactance are computed in different slip rates.

Step 3: Initial value setting: The initial value of equivalent circuit parameter can be found by (21) to (24).

Step 4: Gradient method: Using (10) to (14) to compute the corrections, and using (15) to (18) to update the parameters until the objective functions have decreased in an acceptable range.

Step 5: Dynamic simulation: Based on the parameters of equivalent circuit of step 4 and rotor speed of step 1, the dynamic performance can be simulated by (25) to (30).

Step 6: Moment of Inertia and Friction Coefficient: The moment of inertia and
friction coefficient can be calculated by (33).
Step 7: Calculation accomplished.

Result and Discussion

This section takes measured data of a three-phase, 4-pole, 1/2 hp, 60 Hz induction machine as an example to evaluate this method. This section takes measured data of a three-phase, 4-pole, 1/2 hp, 60 Hz induction machine as an example to evaluate this method. Because its speed varies from the static state to the rating state within one second, it is suitable that sampling rate and sampling number are set as 8192 s/sec and 8192 individually. This method acquires the signals of current, voltage, and speed within this second. And the analysis results are illustrated as follows.

The first part illustrates the required time-varied parameters for analysis. The second part shows the accuracy of initial value setting. The third part interprets the estimation result for equivalent circuit parameters. The fourth part compares the signals of dynamic simulation with measured ones. Finally, the last part discusses the analyzed result of the mechanical parameters.

A. Time-varied Parameter

Fig. 4 shows curves of the voltage, current, and rotor speed in the starting stage of an induction machine [15-16]. The voltage produces some drops in the primary stage, and gradually returns to normal along with the rotor speed increasing. In the primary stage, a larger current cause from the induced voltage of the rotor has not developed. When the rotor speed is near the synchronized state, the current descends to a small value. The phase of impedance changes between 30° and 70°. The reactance is larger than resistance in the primary stage and steady stage. When the rotor speed is near the rated speed, the resistance is larger than reactance.

![Fig. 4 Time-varied parameters](image)

B. Initial value Setting

Fig.5 shows the impedance under different slip rates. It includes variables of resistance and reactance of the induction machine from static state to the rate speed. Curves of resistance and reactance correspond to these in Fig.2.

![Fig. 5 Impedance comparison under different slip rate](image)

It demonstrates that the effect of transient item is
small enough to be ignored in the primary starting stage, and a steady item can offer an accurate and simple result. Based on (21) to (24), the induction machine parameters can be found as $R_s=23.37\Omega$, $R_r=8.68\Omega$, $X_s=13.52\Omega$, $X_r=13.52\Omega$, and $X_m=335.52\Omega$. Curves of resistance and reactance which are simulated by found initial values are also shown in Fig. 5. It shows that a close result can be obtained by the initial values.

C. Parameter of Equivalent Circuit

This paper uses the gradient method to decrease the objective functions to minimum. Because initial values are close to the real ones, the convergence and efficiency of the gradient method will be promoted. Table I shows results of the gradient method. After 4000 iterations, the objective function has reached a minimum. In this case, the disturbance and nonlinearity exists in the practical system, so the objective functions can’t attain zero.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial</th>
<th>Gradient method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1st iteration</td>
<td>2nd iteration</td>
</tr>
<tr>
<td>$R_s$</td>
<td>23.37</td>
<td>23.37</td>
</tr>
<tr>
<td>$R_r$</td>
<td>8.68</td>
<td>8.68</td>
</tr>
<tr>
<td>$X_s$</td>
<td>13.52</td>
<td>13.54</td>
</tr>
<tr>
<td>$X_r$</td>
<td>13.52</td>
<td>13.55</td>
</tr>
<tr>
<td>$X_m$</td>
<td>335.52</td>
<td>335.40</td>
</tr>
<tr>
<td>$E_R (\times 10^3)$</td>
<td>8.0</td>
<td>8.0</td>
</tr>
<tr>
<td>$E_V (\times 10^5)$</td>
<td>22.9</td>
<td>22.7</td>
</tr>
</tbody>
</table>

D. Dynamic Simulation

From the results, this paper simulates the dynamic system with found parameters and compares result with the real one. The simulated result is shown in Fig. 6. The figure shows the comparison of current. The standard deviation of current is 0.241(A). It shows that both of them are quite near. From the result of step 4, the instantaneous has descended to a very small value in one cycle, and then the current presents steady state in Fig. 6. It proves that the steady item holds the variance of current. Figure 6 also shows the dynamic performance of parameters from the standard tests. The standard deviation of current is 0.325(A). It can be found that parameters from this proposed method are more accurate than those from the standard tests.

E. Moment of Inertia and Friction Coefficient

Based on (33) the mechanical parameters can be found as $J=0.38\ (g\cdot m^2)$, and $B=0.61\ (mN\cdot m/(rad/sec))$. Fig. 7 shows the comparison of rotor speed. The standard deviation of rotor speed is 8.388 (rad/sec), which has reached to the minimum. It proves that parameters found by this method are corresponding to the practical.
**Conclusion**

This paper uses time-varied voltage, current and rotor speed to compute the equivalent circuit parameters of an induction machine. Based on the curve of resistance and reactance, the user can obtain the machine’s equivalent circuit parameters. By the found parameters of equivalent circuit and rotor speed, the user can simulate the dynamic performance and obtain the torque, and from the torque and rotor speed, the user can estimate the mechanical parameters. The accuracy of the above steps has been demonstrated. Then, by the measured data of the starting period, the parameters of the induction machine can be obtained, and the user can completely master the operation.

**Reference**


A theory to guide family caregivers of people who are at risk of suicide

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Abstract

Suicide is a major public health problem in Taiwan. All members of the population play a role in the prevention of suicide including families and carers of those at risk. Evidence is sparse on the role that families take in caring for members who have been discharged from hospital following a suicide attempt. The aim of this study was to develop a theory to guide family caregivers of people who are at risk of suicide. Using a grounded theory were used, one-to-one tape-recorded interviews were conducted with patients who had just been discharged from hospitals following a suicide attempt (n=15) and family members (n=15). Data was analyzed using open, axial and selective coding. The core category that emerged was “Impending burn out”, depicting family members’ experience of caring for people who had attempted suicide. Other key categories linked to and embraced within this core category were: On guard day and night, maintaining activities of daily living and creating a nurturing environment. Family caregivers could use the emergent theory as a guide to caring for people at risk of suicide. Psychiatric nurses could use the theory as a framework to educate family members on enhancing the quality of care provided to this group of people. The theory could go some way towards reducing suicidal attempts and decreasing re-hospitalization rates.

Key words: family caregivers, home care, suicide
Introduction

Internationally, epidemiological trends show that there has been a rapid increase in suicide rates in some eastern countries, including Republic of Korea (13.6/100,000 in 2000; 31.0/100,000 in 2009) and Japan (24.1/100,000 in 2000; 24.4/100,000 in 2009). However, there has been a slow decrease in suicide rates in some western countries, including Germany (13.5/100,000 in 2000; 11.9/100,000 in 2006) and Australia (12.5/100,000 in 2000; 8.2/100,000 in 2006) (World Health Organization, 2012). Official statistics demonstrated that suicide rate in Taiwan have increased from 6.2/100,000 in 1993 to 19.3/100,000 in 2006. In response to this situation, the Department of Health in Taiwan launched the Taiwan Suicide Prevention Center in 2005 and set up a suicide report format in order to reduce the high suicide rate in 2006. Finally, suicide was the 11 leading cause of death overall but the second principal cause of death for 15-24 year-olds in 2010 (Department of Health, Taiwan, ROC, 2012).

Evidence demonstrates that there is a particularly high risk of suicide following discharge from hospital. Deisenhammer et al. (2007) used a sample of patients who had been discharged from hospital (n= 665). Findings revealed that 12.8% of the sample group died by suicide on the day of their discharge, 28.4% took their life within seven days of discharge and 47.7% within one month following discharge. Clearly, there are unmet needs in terms of risk assessment prior to discharge. Other evidence illustrates that family members were worried about how they might care for suicidal people (Tzeng & Lipson, 2004). However, there is a lack in research that examines the care that is provide by family members of people who are suicide prone and to date, no theory has been developed to guide families to give proper care to those who are at a high risk of suicide. The current study aimed to redress this gap in knowledge by investigating suicidal ex-patients’ and their families’ perceptions of caring for this group of people at home, and to develop a theory to guide family caregivers of people who are at risk of suicide.

Methods

Study design

Grounded Theory (GT) was considered to be the most appropriate method to use, as the research concerned an experience (suicide), the phenomenon in question was a process (home care) and the goal was the development of theory (Denzin & Lincoln, 2000). Moreover, GT offers a rigorous method for undertaking qualitative research (Strauss & Corbin, 1994; Wainwright, 1994). Further, it is not simply descriptive, its primary purpose being to generate explanatory theories of human behaviour (Morse & Field, 1996).

Sample

A purposive sampling technique was used initially, and then theoretical sampling guided the selection of further participants (Williams, 1998). Two hospitals in Taiwan granted access...
to the patient and family sample. The patient sample was restricted to those having had suicidal ideations for two weeks prior to data collection or having had a previous suicide attempt(s). The family sample was restricted to those members of the family who were caring for their relatives after they had been discharged from hospital for at least three days. The final number of participants was 30, comprising ex-patients (n=15) and their family members (n=15). Following consent their family members were then approached and informed about the study. The patients comprised twelve women and three men, fourteen of whom had been diagnosed with depression and one with schizophrenia. Two were admitted with suicidal intention and were considered to be at risk of completing suicide. The remaining 13 were admitted as a result of overt suicidal behaviour, for example, drug overdose, or severe wrist cutting. The families were nine men and six women. Their relationships with the ex-patients were: partners (n=6), parents (n=4), siblings (n=3), children (over the age of 20) (n=2). The periods of care, at home, after discharge ranged from 3-42 days.

Data collection

Interviews took place in a quiet room in the hospitals (n=18) and in the families’ homes (n=12) and lasted approximately 60 minutes. All patients had been discharged from hospitals for at least one week. The initial interview guide for patients contained the following questions: (1) how has this week been for you; (2) in what ways do your family members care for you; (3) how do you expect your family to care for you; (4) do you have any outside help; (5) how do you feel about your home and family; and (6) why do you think people attempt suicide? The questions in the initial interview guide for family members were: (1) What has it been like for you to care for [name] at home; (2) in what way do you communicate with [name]; (3) Tell me about the difficulties you have experienced; (4) how do you cope with these difficulties; (5) do you receive any outside help; (6) how would you describe your relationship with [name]; and (7) why do you think people attempt suicide?

Ethical considerations

The research proposal was approved by the two hospitals’ ethics committees and each participant was informed of the purpose of the research and a consent form was signed. Several steps were taken to protect participants from harm:

1. Rigorous criteria for selection and exclusion included a psychiatrist assessing patients to determine their fitness to participate.
2. The consent process was ongoing.
3. Interviews were conducted when patients felt able and willing to share their feelings and thoughts about their suicidal ideations and/or suicide attempts.
4. Confidentiality was maintained by using codes to identify participants.

Data analysis

In grounded theory, data collection, coding and analysis are simultaneous processes from the
beginning of a study to its conclusion (Strauss & Corbin, 1990). In the current study, data were analysed using a synthesis of the Strauss and Corbin (1998) analytical framework, comprising open, axial and selective coding, together with Eaves’ (2001) 12 analytical steps to increase understanding and enhance the clarity of grounded theory data analysis. In addition, the QSR NUD*IST, N7 software program was used to aid the coding, sorting, and retrieval of data (Gahan & Hannibal, 1998).

Stage 1: Open coding
After each participant’s data were collected and the taped interviews were typed, the researcher began the data analysis using line-by-line in-vivo coding to capture the main idea of what the informants said coding it into significant statements (meaningful units) the concepts emerged. Then, similar concepts were grouped together to develop categories by using the constant comparative method. Subsequently, categories were developed in terms of their properties and dimensions and further differentiated by breaking them down into subcategories.

Stage 2: Axial coding
This was used to link each category within the paradigm which included causal conditions, contextual conditions, intervening conditions, action/interactions, and consequences. In this step, the researcher reflected on and examined relationships in the data by using the constant comparison technique.

Stage 3: Selective coding
The core category is identified and all other categories can be related to the core category. The core category led to the discovery of the basic social psychological process and then a substantive theory was generated from the data to guide family caregivers of people who are at risk of suicide.

Findings

Twelve categories emerged from the data and relationships were identified using Strauss and Corbin’s (1998) paradigm model. The basic components of the paradigm model are the causal conditions, context, intervening conditions, action/interaction strategies, and consequences. A substantive theory was then developed entitled “A theory to guide family caregivers of people who are at risk of suicide” (see Figure 1). The way in which each of the properties within the paradigm model interacts with each other, and, in turn, how each relates to development of the core category are detailed in the diagram and examined below.

Causal conditions
The causal conditions represented sets of events or happenings that influenced the phenomenon of suicide (Strauss & Corbin, 1998). In order to carry out their role effectively, family members and carers needed to be aware of the causal conditions which could have led people to attempt suicide. Three categories were generated relating to the causal conditions and these were then reduced to seven subcategories (Table 1).
Generally, the findings showed that there were many reasons why these patients had suicidal ideations and why some attempted suicide. Specifically, ex-patients described an inability to cope with life, coupled with having to endure a range of painful experiences. Their thoughts prior to the suicide attempt influenced the degree of seriousness of the attempt and the type of self-destructive behaviour they embarked on to communicate their pain. The following two citations illustrate these feelings:

Patient 10 (P 10): Many things continue to torture
me and I suffer from tunnel vision; this means that I have no aim in life. I feel life is meaningless.

Family 7 (F7): People who want to commit suicide are suffering from many painful things. The painful things take over their thinking until there is nothing left to think about.

<table>
<thead>
<tr>
<th>Table 1 Causal conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Subcategories</strong></td>
</tr>
<tr>
<td>Stress-history and past trauma</td>
</tr>
<tr>
<td>Illness</td>
</tr>
<tr>
<td>Feelings of abandonment</td>
</tr>
<tr>
<td>Decrease in suicidal ideas</td>
</tr>
<tr>
<td>Increase in suicidal ideas</td>
</tr>
<tr>
<td>Pre-suicidal clinical features</td>
</tr>
<tr>
<td>Attempted suicide</td>
</tr>
</tbody>
</table>

**Context**

Contextual conditions, according to the paradigm model, related to the specific sets (patterns) of conditions that intersected at this time and place to create a set of circumstances or problems through which the participants responded through their actions/interactions (Strauss & Corbin, 1998). Two categories were generated relating to contextual conditions, and these and their subcategories are shown in Table 2.

Table 2 demonstrates that, in the context component of the paradigm model, hospital patients were discharged to receive care from their families or carers following a suicide attempt. The family environment and Chinese culture impacted on the family members who were primarily caring for their relatives, some who were continuing to have suicidal ideas. The findings illustrated that the participants’ perceived the family setting to be a hazardous situation because it was an open environment, thus they could not manage to monitor the whereabouts and behaviours of their relatives at risk of suicide. Moreover, the relationship dynamics in the family coupled with their mood affected the quality of their ability to care. Further, the family members felt a collective shame about one of their members attempting suicide mainly because the Chinese culture deems suicide as a stigma. These factors affected the family, hence they attended folk therapy rather than seeking help from hospitals. The following two narratives illustrate these findings:

P 8: I went upstairs to write my will then I went downstairs to attempt suicide. My family

<table>
<thead>
<tr>
<th>Table 2 Contextual conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Subcategories</strong></td>
</tr>
<tr>
<td>Hazardous family setting</td>
</tr>
<tr>
<td>The family’s relationship</td>
</tr>
<tr>
<td>The family’s mood</td>
</tr>
<tr>
<td>Stigma</td>
</tr>
<tr>
<td>Folk therapy</td>
</tr>
</tbody>
</table>
tried to stop me but they couldn’t because I got on my motorcycle and went to Love river and tried to commit suicide by drowning.

F 3: A neighbour is very nice and she often chats with me. But I could never talk with her about my daughter’s suicide attempt because I feel so ashamed.

**Intervening conditions**

The intervening conditions were the broader structural context pertaining to the phenomenon of suicide. These conditions act either to facilitate or constrain the action/interactional strategies taken within a specific context (Strauss & Corbin, 1990). Two categories emerged relating to the intervening conditions. These and their subcategories are shown in Table 3.

<table>
<thead>
<tr>
<th>Subcategories</th>
<th>Categories</th>
</tr>
</thead>
<tbody>
<tr>
<td>Support systems</td>
<td>Effects of caring</td>
</tr>
<tr>
<td>Families’ coping strategies</td>
<td></td>
</tr>
<tr>
<td>Lack of support systems</td>
<td></td>
</tr>
<tr>
<td>Caring difficulties</td>
<td>Barriers to caring</td>
</tr>
<tr>
<td>Families’ caring ability problems</td>
<td></td>
</tr>
</tbody>
</table>

**Action/interaction strategies**

The action/interaction strategies were purposeful or deliberate acts which were taken to resolve a problem and which shaped the phenomenon in some way (Strauss & Corbin, 1998). In this study, three categories were generated in the action/interaction strategies component of the paradigm model (see Table 4). During the process of care, family members experienced overlapping and dynamic degrees of action and interaction among the three categories.

The first category “On guard day and night” helped to ensure that their relatives felt safe. The second category “maintaining activities of daily living” promoted physical recovery. The third category “creating a nurturing environment” facilitated mental health healing. Three examples demonstrate how the family members provided care:

P3: My mother pays attention to my safety all the time. She worries about me committing suicide if I come home late.
F9: I prepare food and tonics for my daughter. Sometimes, I stew ginseng and fish with medlar [a tonic] for her in order to make her feel physically healthier.

P9: My family always focuses on what I’m doing and how I’m feeling. They keep asking me “what’s wrong with you” when I’m very quiet.

Table 4 Action/interaction strategies

<table>
<thead>
<tr>
<th>Subcategories</th>
<th>Categories</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paying attention to observation</td>
<td>On guard day and night</td>
</tr>
<tr>
<td>Paying attention to patients’ safety</td>
<td></td>
</tr>
<tr>
<td>Providing Physical care</td>
<td>Maintaining activities of daily living</td>
</tr>
<tr>
<td>Providing treatment</td>
<td></td>
</tr>
<tr>
<td>Arranging activities</td>
<td></td>
</tr>
<tr>
<td>Caring and support</td>
<td></td>
</tr>
<tr>
<td>Fostering tranquility</td>
<td></td>
</tr>
<tr>
<td>Re-awakening hope</td>
<td></td>
</tr>
</tbody>
</table>

Consequences

The consequences result from the action/interaction strategies and are the final aspects of the paradigm model (Strauss & Corbin, 1998). In this study, two categories emerged relating to the consequences (See Table 5). Table 5 shows that, when family members carried out action/interaction strategies related to providing care for their relatives at risk of suicide, the positive consequence that emerged demonstrated that the ex-patients regained the desire to live. The negative consequence that emerged related to the ex-patients holding on to their recurrent suicidal thoughts and sometimes, making further suicide attempts. These bi-polar consequences are illustrated in the following narratives.

P 4: I haven’t had any suicidal ideas for three weeks because I make sure I take my medicine punctually.

F13: She’s attempted suicide twice by cutting her wrists since she was discharged from hospital.

Table 5 Consequences

<table>
<thead>
<tr>
<th>Subcategories</th>
<th>Categories</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elimination of suicidal thoughts</td>
<td>Regaining the desire to live</td>
</tr>
<tr>
<td>Improved health and well-being</td>
<td></td>
</tr>
<tr>
<td>Recurrent suicidal thoughts</td>
<td>Recurrent suicidal thoughts and attempts</td>
</tr>
<tr>
<td>Re-hospitalisations</td>
<td></td>
</tr>
</tbody>
</table>

Core category

The core category was the central phenomenon around which all the other categories were integrated (Strauss & Corbin, 1998). In the current study, nine patients had attempted suicide more than five times before they were discharged from hospital. Three patients had attempted suicide twice since their latest discharge from hospital. It emerged from the findings that their family members had to spend twenty-four hours per day worrying about them and providing all round care for them. Therefore, the core category that emerged was “Impending burn out” as the family members perceived that they were both...
physically and emotionally exhausted. The following narratives depict these findings:

P15: In fact, it’s more painful to take care of us than to take care of people who are disabled because our emotions are so unstable. Our families need a lot of patience.

F3: I feel so stressed when caring for my daughter because I’m always thinking: ‘is she safe today? Will she cut her wrist? Does she want to die?’ If she has a problem, I worry about her all day long.

Discussion

The components of the paradigm model helped to define some of the complex relationships among the conditions and the importance of the family’s relationship with their suicidal relative (see Figure 1). The findings demonstrate that family caregivers have a pivotal role in caring for their relatives after they have been discharged from hospital. Therefore, the substantive theory that was developed is a very complex and detailed account of a suicide family care theory, which could be used as a foundation upon which to design and deliver a psychoeducation suicide care programme for family caregivers of people who are at risk of suicide.

In relation to the causal conditions, findings revealed that people attempt suicide because they cannot cope with life. In the current study, 12 of the 15 patients who had attempted suicide had taken drug overdoses or cut their wrists. These findings correspond with results found in Modai et al.’s (2002) research. They interviewed a sample of in-patients (n=250). The results indicated that the methods used in previous suicide attempts were as follows: drug overdose (33.8%), hanging (20.5%), cutting or stabbing (17.6%) and gun shot wounds (2.9%). Researchers argue that the level of ‘intent-to-die’ could be assessed by focusing on the different methods individuals use to attempt suicide (Galloucis & Francek, 2002).

Findings from the current study revealed that participants deemed suicide a stigma. These findings support those of Tzeng and Lipson (2004) who found that patients and families suffer postsuicide stigma following an attempt. The Taiwanese government aim to reduce the stigma associated with suicide via the media, which plays a vital role in providing information about the impact of suicide (Tousignant et al. 2005). For example, media reporting can have an impact on copycat suicides. Conversely, the media can also transmit knowledge relating to pain, empathy and compassion, which could help change people’s attitudes toward the stigma related to suicide. Further, the media could help to direct people and the families towards mental services rather than folk therapy when they are at high risk of suicide (Lee et al. 2007).

In Chinese society, family caregivers play a significant role in the treatment of mentally ill patients at home because of Chinese expectations and obligations (Tung & Gillett, 2005). However, this study found that the family members only provided twenty-four-protection for their relatives because they lacked the knowledge required to provide further care. These findings corroborate
the results of Su’ (2003) study and showed that 31.9% of the primary caregivers had received knowledge from hospital staff on preventative strategies relating to suicide. Moreover, the results indicated that 66.8% of the caregivers had not noticed any ‘abnormal behaviours’ prior to their relatives attempting suicide. Therefore, it is crucial for nurses to educate family members on a range of suicide preventative strategies.

Moreover, the current study found that family members spend more time providing physical care for the ex-patients than mental health care. These findings support those of Su (2003), who found that family members used the following preventative strategies. The family members; sent their relatives to hospital quickly when their ‘condition changed’; helped with treatment and follow-up appointments; tried to ensure compliance with medication; were concerned about their sleep patterns. However, both the findings from the current study along with those of Su (2003) illustrate that family members were unaware of how to cope with the mental health impact associated with the attempt or with the mental illness which many of the ex-patients had been diagnosed as having. It is vitally important that hospital staff provide psycho-education programmes to families on these topics. Other subjects, which could be included are: attitudes to mental illness, suicide and the aftermath of suicide on families, carers and the community. These psycho-education programmes of care could have a role in reducing people’s suicidal ideas.

**Limitations**

This study had three main limitations. First, the difficulties involved in collecting data from suicidal patients and their families in Taiwan because of the collective, cultural shame experienced regarding suicide. Consequently, it took one year to collect the data. Second, data was collected within six weeks following the patient’s discharge. In future research, data could be collected at different time points following the patient’s discharge to explore different caring experiences. Third, only three of the 15 ex-patients were males because women are twice more likely to attempt suicide than men in Taiwan (Department of Health, Taiwan, ROC, 2012).

**Conclusion**

The findings of this study were grounded in the experience of family members caring for ex-patients who had recently been discharged from hospital following a suicide attempt. The lived experiences of the ex-patients were also collected. In keeping with one of the axioms of grounded theory a suicide care theory emerged from the data. To date, this is the fist theory, which families and carers could use as a map to guide them when caring for people at risk of suicide. Psychiatric nurses could use this theory as guide to provide information to family members prior to their relatives being discharged from hospital. Nurses have a key role in teaching family members on providing care for people who are at risk of suicide. One of our intentions is to stimulate further discussion and new research on the topic.
of suicide and the care of suicidal patients who had just been discharged from hospital with the aim of reducing their recurrent suicide thoughts and attempts.

References

cultural context of suicide stigma in Taiwan. Qualitative Health Research 14, 345-358.


Derivation of Equations for the Electromagnetic Interactions between Molecular Solutes

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Abstract

As the rapid progress of molecular biology and nanotechnology, the development of theoretical and computational science is toward to exploration of the electromagnetic interactions between solutes with nanometer dimension. How to treat Avogadro’s number of solvent molecules has become a challenge. Until now, two ways were developed to treat the solvent effect. One is molecular dynamics (MD) simulation, but MD simulation cannot mimic Avogadro’s number of solvent molecules. The other one uses Maxwell’s equations. Maxwell’s equations were developed for treating the Avogadro’s number of polarized/magnetized molecules in materials, but not for the electromagnetic interactions between molecular solutes. Therefore, the equations were derived by combining statistical thermodynamics, Coulomb’s law, Biot-Savart law and Faraday’s law of induction. The solutions from the derived equations have the following characteristics:

1. the solvent dielectric polarization behaves oscillation as distance to solute as observed from MD simulations.
2. The derived equations can treat the time-dependent electromagnetic interactions as Maxwell’s equations do.
Keywords: solvation free energy, protein-protein/ligand interactions, external electric field, nonthermal effect

Introduction

Electromagnetic force is one of the four fundamental interactions in Nature.\textsuperscript{1,2} Gauss’s law, Ampere’s law, and Faraday’s law of induction can be used to compute the electromagnetic interactions between charged particles in vacuum. In materials, it is almost impossible to evaluate the electromagnetic field by treating the numerous polarized/magnetized molecules as sources. Hence, Maxwell treated the electric/magnetic effect of discrete polarized/magnetized molecules as an uniform distribution of electric/magnetic dipole moments, $p/m$, and assumed the induced electric/magnetic dipole moment per unit volume, $P/M$, to be proportional to the electric/magnetic field, $E/B$. By space-averaging $E$ and $B$ over a region containing thousands of atoms,\textsuperscript{1} a set of equations that describes the electromagnetic interactions between the charged particles in materials was derived.\textsuperscript{1,2}

However, Maxwell’s equations cannot treat the electromagnetic interactions between solutes with nanometer dimension. Such interactions can be found in nanotechnology\textsuperscript{3}, bioelectromagnetism\textsuperscript{4,5}, and biological systems\textsuperscript{6-7}. In Maxwell’s equations, the solvent density $\rho$ was assumed as the bulk solvent density $N_{\text{bulk}}$\textsuperscript{1,2}, but $\rho$ near a solute differs dramatically from $N_{\text{bulk}}$\textsuperscript{8-9}. And the dielectric polarization $P$ averaged over a macroscopic region from Maxwell’s equations cannot replace the electromagnetic effects from near-solute structured solvent. Though, continuum models are widely used to compute hydration free energies of molecules\textsuperscript{10-11}. As the progress in observational technologies, one of the major concerns is how to incorporate the electromagnetic effects of the near-solute solvent and treat the electromagnetic interactions between molecular solutes in a macroscopic system.

Although the methods such as quantum mechanics, MD and Monte-Carlo simulations can capture the microscopic features of the near-solute solvent molecules\textsuperscript{12-13}, they cannot treat time-dependent electromagnetic fields and Avogadro’s number of solvent molecules. Hence, the equations were derived that can capture the near-solute $\rho$ and solvent dielectric polarization $P$ as in MD simulations, and can treat time-dependent electromagnetic interactions and macroscopic systems just like Maxwell’s equations do. Here $P$ was described as the product of the solvent molecular density $N_{\text{bulk}}g$, and the dipole moment per solvent molecule averaged over a period time $p$, as $P = N_{\text{bulk}}gp$. The $g$ and $p$ can be computed from the mean force $F$ and electric field $E$ acting on a solvent molecule, respectively. And the $F$ and $E$ can be computed from $g$ and $P$. The equations governing the relation among $g$, $F$, $p$, $P$ and $E$ were introduced.

Theory

Relationship between $g(r)$ and $F(r)$. Consider a solute immersed in $n$ solvent molecules. Each solvent molecule has three translational and rotational degrees of freedom. The probability of finding $n$ solvent molecules at positions
\((r_1, r_2, \ldots, r_n)\) with Euler angles \((\Omega_1, \Omega_2, \ldots, \Omega_n)\) and the solute atom at \(r_{\text{solute}}\) follows a Boltzmann distribution, \(\exp[-U(r_{\text{solute}}, r_1, \ldots, r_n, \Omega_1, \ldots, \Omega_n)/k_B T]/Z_n\), where \(U\) is the interaction potential energy, \(k_B\) is Boltzmann’s constant, \(T\) is the absolute temperature, and \(Z_n\) is the partition function.

\[
Z_n = \int \cdots \int \exp \left[ -\frac{U(r_{\text{solute}}, r_1, \ldots, r_n)}{k_B T} \right] \ dr_1 \cdots dr_n \Omega_1 \cdots \Omega_n \tag{1}\]

The probability of finding a solvent molecule at \(r_1, g(r_1)\), is given by:

\[
g(r_1) = \frac{1}{Z_n} \int \cdots \int \exp \left[ -\frac{U(r_{\text{solute}}, r_1, \ldots, r_n)}{k_B T} \right] \ dr_1 \cdots dr_n \Omega_1 \cdots \Omega_n \tag{2}\]

By taking the gradient of \(g(r_1)\) relative to \(r_1\), \(g(r)\) is related to the mean force–\(F(r)\), acting on the solvent molecule by:

\[
\nabla g(r)/g(r) = F(r)/k_B T \tag{3}\]

and, \(g(r)\) is related to \(F(r)\) by:

\[
g(r) = g(\infty) \exp \left[ \int_{\infty}^{r} F(r') \cdot dr'/k_B T \right] \tag{4}\]

where \(g(\infty)\) is the relative solvent molecular density at an infinite distance from the solute.

**Relationship between \(p(r)\) and \(E(r)\).** Consider a solute immersed in \(n\) solvent molecules. Each solvent molecule has three translational and rotational degrees of freedom. The probability of finding \(n\) solvent molecules at positions \((r_1, r_2, \ldots, r_n)\) with Euler angles \((\Omega_1, \Omega_2, \ldots, \Omega_n)\) and the solute atom at \(r_{\text{solute}}\) follows a Boltzmann distribution, \(\exp[-U(r_{\text{solute}}, r_1, \ldots, r_n, \Omega_1, \ldots, \Omega_n)/k_B T]/Z_n\), where \(U\) is the interaction potential energy, \(k_B\) is Boltzmann’s constant, \(T\) is the absolute temperature, and \(Z_n\) is the partition function (1). The probability of finding a solvent molecule at position \(r_1\) with orientation angle \(\Omega_1, g(r_1; \Omega_1)\), is given by:

\[
g(r_1; \Omega_1) = \frac{1}{Z_n} \int \cdots \int \exp \left[ -\frac{U(r_1)}{k_B T} \right] \ dr_1 \cdots dr_n \Omega_1 \cdots \Omega_n \tag{5}\]

By taking the gradient of \(g(r_1; \Omega_1)\) relative to the orientation \(\Omega_1\), the relationship between \(\nabla_{\Omega_1} g(r_1; \Omega_1)\) and \(g(r_1; \Omega_1)\) can be found as;

\[
\nabla_{\Omega_1} g(r_1; \Omega_1)/g(r_1; \Omega_1) = \tau_{1, \text{mean}} (r_1; \Omega_1)/k_B T \tag{6}\]

Where the mean torque \(\tau_{1, \text{mean}}(r_1; \Omega_1)\) was defined as;

\[
\tau_{1, \text{mean}} (r_1; \Omega_1) \equiv \int \cdots \int -\nabla_{\Omega_1} U \exp\left[-U/k_B T\right] dr_1 \cdots dr_n \Omega_1 \cdots \Omega_n \tag{7}\]

The probability of the solvent molecule being at \((r; \Omega)\) can be calculated from the probability of the solvent molecule being at \((r; \Omega_{\text{ref}})\) and the mean torque along the path from \(\Omega_{\text{ref}}\) to \(\Omega\) as;

\[
g(r; \Omega) = g(r; \Omega_{\text{ref}}) \exp \left[ \frac{1}{k_B T} \int_{\Omega_{\text{ref}}}^{\Omega} \tau_{\text{mean}} (r; \Omega') \cdot d\Omega' \right] \tag{8}\]

For the solvent molecule at \(r\), the probability to find the solvent molecule at orientation \(\Omega\) can be calculated as \(g(r; \Omega)\) divided by the integral of \(g(r; \Omega)\) over all orientations as;

\[
\Omega(r; \Omega) = g(r; \Omega)/\int g(r; \Omega'n) d\Omega'n. \tag{9}\]

Defining the potential of mean torque \(U_{\text{mean}}g(r; \Omega)\) as;

\[
U_{\text{mean}} (r; \Omega) \equiv -\int_{\Omega_{\text{ref}}}^{\Omega} \tau_{\text{mean}} (r; \Omega') \cdot d\Omega', \Omega(r; \Omega) \text{ is;}
\]
\[ \Omega(r, O) = \frac{\exp[-U_{\text{mean}}(r, O)/k_B T]}{\int \exp[-U_{\text{mean}}(r', O)/k_B T] dO'} \] (9)

The electrical effect of a solvent molecule modeled as a point dipole moment \( \mu \), \( p(r) \) can be calculated as the integral of \( \mu(r, \theta, \phi) \) weighted by \( \Omega(r, \theta, \phi) \) over all orientations;

\[ p(r) = \int_0^{2\pi} \int_0^\pi \mu(r, \theta, \phi) \Omega(r, \theta, \phi) \sin \theta d\theta d\phi \] (10)

In a pure solvent system, or in a region far away from the solute, \( p(r) \) is proportional to \( E(r) \) as,

\[ p(r) \approx \frac{\mu^2 E(r)}{3k_B T} = \varepsilon_0 \gamma_{\text{mol}} E(r) \] (11)

where solvent molecular polarizability \( \gamma_{\text{mol}} \) was defined as the ratio between \( p \) and \( (\varepsilon_0 E)^2 \).

**Relationship between \( E(r) \) and \( P(r) \).** The \( E \) was contributed from the solute with charge \( \rho_{\text{free}}(r') \) and the perturbed dielectric polarization \( P'(r'; x) \) as;

\[ E(r) = -\int \left[ \rho_{\text{free}}(r') \right] \nabla \frac{1}{4\pi \varepsilon_0 R} d^3 r' \] (12)

where \( R \) is the distance between the solvent at \( r \) and the solute charge or solvent dielectric polarization at \( r' \).

The perturbed \( P'(r'; x) \) was the dielectric polarization \( P(r') \) perturbed by the solvent molecule at \( r \), and can be written as \( \rho_{\text{bulk}} g'(r'; x) p(r', x) \), where \( g'(r'; x) \) is the perturbed solvent density, and \( p(r', x) \) is the perturbed solvent dipole at \( r' \), due to the solvent dipole at \( r \). The perturbed \( g'(r'; x) \) can be approximated by the unperturbed \( g(r') \) scaled by a Heaviside/unit step function, \( g'(r'; x) \approx u(R - Rc) g(r') \), where \( Rc \) is the solvent radius. Assume that \( p(r'; x) \sim p(r') \), (12) can rewritten as;

\[ E(r) = \varepsilon_0 E(r) - \int \left[ \nabla \cdot \left( \rho_{\text{free}}(r') \right) \right] \nabla \left( \frac{1}{4\pi \varepsilon_0 R} \right) d^3 r' \] (13)

**Derivation of Microscopic Gauss’s Law.**

Microscopic Gauss’s Law is obtained by taking the divergence of \( E \) in (13) and defining the microscopic electric displacement \( D \) such that its divergence is the solute charge density, \( \nabla \cdot D = \rho_{\text{free}} \). Whereas \( D \) is related to \( E \) in microscopic Gauss’s Law by;

\[ D(r) = \varepsilon_0 E(r) - \int \left[ \nabla \cdot P'(r', r) \right] \nabla \left( \frac{1}{4\pi \varepsilon_0 R} \right) d^3 r' \] (14)

Ampere law of microscopic electrodynamics is obtained by replacing the macroscopic \( D \) in Ampere law of Maxwell’s equation \( \nabla \times H = J + \partial D/\partial t \) with the microscopic \( D \) in (14). It relates the microscopic magnetic field \( H \) to the electric current \( J \) and the microscopic \( D \). The differences between the macroscopic and microscopic electrodynamics equations are summarized in Table 18.
### Table I. Macroscopic vs. Microscopic Electrodynamics equations

<table>
<thead>
<tr>
<th>Maxwell’s equations</th>
<th>Microscopic electrodynamics equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gauss’s law</td>
<td>$\nabla \cdot \mathbf{D} = \rho_{\text{free}}$</td>
</tr>
<tr>
<td></td>
<td>$\nabla \cdot \mathbf{B} = 0$</td>
</tr>
<tr>
<td>Faraday’s law of induction</td>
<td>$\nabla \times \mathbf{E} = -\partial \mathbf{B} / \partial t$</td>
</tr>
<tr>
<td>Ampere-Maxwell’s law</td>
<td>$\nabla \times \mathbf{H} = \mathbf{J} + \partial \mathbf{D} / \partial t$</td>
</tr>
<tr>
<td>Electric displacement field, $\mathbf{D}$</td>
<td>$\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}$</td>
</tr>
<tr>
<td>Magnetic field, $\mathbf{H}$</td>
<td>$\mathbf{H} = \mathbf{B} / \mu_0 - \mathbf{M}$</td>
</tr>
<tr>
<td>Dielectric polarization, $\mathbf{P}$</td>
<td>$\mathbf{P} = \varepsilon_0 \chi_e \mathbf{E}$</td>
</tr>
<tr>
<td>Magnetic dipole density, $\mathbf{M}$</td>
<td>$\mathbf{M} = \chi_m \mathbf{g} \mathbf{B} / \mu_0$</td>
</tr>
<tr>
<td>Solvent molecular density, $g$</td>
<td>$g = 1$</td>
</tr>
<tr>
<td>Lorentz force, $\mathbf{F}$</td>
<td>$\mathbf{F} = q(E + v \times \mathbf{B})$</td>
</tr>
</tbody>
</table>

$F_{\text{vdW}}$: van der Waals force; $\mathbf{J}$: free current density; $\mathbf{P}'$: perturbed electric dipole density; $q$: charge of the particle; $v$: velocity of the particle; $\chi_e$: electric susceptibility; $\chi_m$: magnetic susceptibility; $\varepsilon_0$: vacuum permittivity; $\mu_0$: vacuum magnetic permeability; $\rho_{\text{free}}$: free electric charge density.

### Methods

**MD simulations.** The simulation system was a one-particle solute at the center of a spherical water cluster of radius of 20 Å containing 1118 TIP3P water molecules. The charge state of the solute ranged from $-1 \text{ e}$ to $+1 \text{ e}$. The van der Waals (vdW) parameters of solutes were assigned the same values as the oxygen atoms of the TIP3P water where $\varepsilon = -0.1521 \text{ kcal/mol}$ and $R_{\text{min}}/2 = 1.7682 \text{ Å}$. Simulations were carried out in an NVE ensemble using the CHARMM package using spherical boundary conditions without cutoffs. The ion–water and water–water interaction energies were calculated by summing the electrostatic and vdW pairwise energies. For the TIP3P water, the charge states of the oxygen and hydrogen atoms were $-0.834 \text{ e}$ and $+0.417 \text{ e}$, respectively. The vdW parameters of the hydrogen atoms are $\varepsilon = -0.046 \text{ kcal/mol}$ and $R_{\text{min}}/2 = 0.2245 \text{ Å}$. The length of the O–H bonds in TIP3P (0.9572 Å), and the angle of the H–O–H bond (104.52°), were constrained during the simulations using the SHAKE algorithm. All atoms were propagated according to Newton’s equations using the leapfrog Verlet algorithm and a time-step of 2 femtoseconds at a mean temperature of 300 K. Each system was first minimized for 1000 steps, equilibrated for 200 picoseconds, and then subjected to 80 nanoseconds of production dynamics. Configurations were stored every 20 femtoseconds.

**Calculate $g(r)$, $p(r)$ and $E(r)$ from the trajectories of the MD simulations.** The radial distribution function $g(r)$ was calculated as the number of water molecules $N(r)$ in the radius of the shell between $(r-\Delta r/2)$ and $(r+\Delta r/2)$ over $N_c$ configu-
rations/frames, divided by the volume enclosed by the radius of the shell between \((r-\Delta r/2)\) and \((r+\Delta r/2)\) over \(N_c\) configurations/frames, with a bulk water density of \(N_{\text{bulk}} = 0.0334/\text{Å}^3\).

\[
g(r) = \frac{N(r)}{4\pi r^2 \Delta r N_c N_{\text{bulk}}} \tag{15}
\]

\(N(r)\) in (15) was computed as the summation of the number of water molecules whose oxygen atom was at a distance from solute of between \((r-\Delta r/2)\) and \((r+\Delta r/2)\).

\[
N(r) = \int_{r-\Delta r/2}^{r+\Delta r/2} \sum_{l=1}^{N_c} \sum_{m=1}^{n} \delta \left( r' - r_{0m}^{lm} \right) dr' \tag{16}
\]

where the first summation is over \(N_c\) configurations/frames, the second summation is over the \(n\) solvent molecules in the simulation system, where \(r_{0m}^{lm}\) denotes the coordinates of the oxygen atom of water molecule \(m\) in configuration \(l\), and \(\Delta r\) is set as 0.1 Å.

The direction of \(p(r)\) was radial. The amplitude of \(p(r)\) was calculated by summing the electric dipole moment of the water molecules with its oxygen atom located between \((r-\Delta r/2)\) and \((r+\Delta r/2)\) over \(N_c\) configurations/frames, divided by the number of water molecules \(N(r)\).

\[
p(r) = \int_{r-\Delta r/2}^{r+\Delta r/2} \sum_{l=1}^{N_c} \sum_{m=1}^{n} \sum_{i=1}^{3} q_i \left( r_i^{lm} \cdot r_{0m}^{lm} \right) \delta \left( r' - r_{0m}^{lm} \right) dr' \tag{17}
\]

where \(q_i\) is the charge of the water atom \(i\), \(r_i^{lm}\) denotes the coordinates of the atoms of water molecules \(m\) in configuration \(l\).

For a one-particle solute with charge state \(Q\), the direction of \(E(r)\) is radial. \(E(r)\) calculated from the trajectories of the MD simulation was,

\[
\delta \left( \frac{q_i}{4\pi (r_{0m}^{lm})^2} \right) + \int_{r-\Delta r/2}^{r+\Delta r/2} \sum_{m=1}^{n} \sum_{l=1}^{N_c} 4\pi \left( \frac{R_{ij}^{lm}}{r_{ij}^{lm}} \right) \delta \left( r - r_{ij}^{lm} \right) dr' \tag{18}
\]

where \(\varepsilon_0\) is the permittivity of free space, \(q_i\) is the charge of the water atom \(i\), \(q_j\) is the charge of the solute atom, \(R_{ij}^{lm}\) is the distance between the oxygen atom of water molecule \(m'\) in configuration \(l\) and the solute \(j\), \(R_{ij}^{lm}\) is the vector from the oxygen atom of water molecule \(m'\) to the atom \(i\) of water molecule \(m\) in configuration \(l\).

Calculate \(g(r)\) and \(P(r)\) from microscopic Gauss’s law. An iterative strategy was used to obtain the \(g\) and \(P\) (Figure 1). Using an initial guess of \(g^{(0)} = 1\) and \(P^{(0)} = q(1-1/\varepsilon)/(4\pi r^2)\) from macroscopic Gauss’s law, the \(E\) acting on the solvent molecule at \(r\) was evaluated using (13) with \(R_c = 2.8\ \text{Å}\). Knowing \(E^{(1)}\) and \(g^{(0)}\), the mean force acting on the solvent molecule at \(r\) can be evaluated. The mean force was used to yield a new \(g^{(1)}\) using (4), which was used together with \(E^{(1)}\) to compute a new \(P^{(1)}\). With the new \(g^{(1)}\) and \(P^{(1)}\) values, the above procedure was repeated until the \(g\) and \(P\) values converged.
Results/Discussions

The performance of calculating $g(r)$ from $F(r)$ using (4). The $g(r)$ obtained indirectly from the mean force was compared with the $g(r)$ obtained directly by counting the number of water molecules from the trajectories of MD simulations. The results in Figure 2 show that the $g(r)$ obtained indirectly from the $F(r)$ can reproduce the respective $g(r)$ obtained by direct counting.

Figure 2. Comparison of $g(r)$ computed from counting directly and mean force. The $g(r)$ was derived from MD simulations of a solute atom of charge $Q$ equal to +1e (solid curves), 0e (dot dashed), and −1e (dashed) in TIP3P water. The black curves correspond to $g(r)$ obtained by direct counting, while the red curves correspond to $g(r)$ obtained indirectly from the mean force using (4).

Figure 3. Comparison of $p(r)$ computed from counting directly and from the electrostatic field. For one-particle solute in TIP3P water cluster, the electric dipole moment $p(r)$ counted from MD simulation directly (black line) and estimated from electrostatic field using (11) (red line) were compared as a function of distance solute for the solute charge $Q = (a) 0e$, (b) +0.2e, −0.2e, (c) +0.4e, −0.4e, (d) +0.6e, −0.6e, (e) +0.8e, −0.8e, (f) +1e, −1e.
The performance of calculating \( p(r) \) from \( E(r) \) using (11). The electric dipole moment \( p(r) \) is proportional to the electrostatic field \( E(r) \) under several assumptions. To understand the performance of calculating \( p(r) \) of TIP3P water molecules from \( E(r) \), \( p(r) \) counted from the trajectories of MD simulations was compared with computed using (11). The results show that the \( 4\pi r^2 N_\text{local} p(r) \) counted from the trajectories of MD simulations was consistent with computed using (11) for solute charge \( Q \) between \(-1 \text{ e} \) and \(+1 \text{ e} \) (Figure 3).

![Figure 4](image)

**Figure 4.** Comparison of \( g(r) \) and \( P(r) \) from microscopic Gauss's law, macroscopic Gauss's law and MD simulations. The (a) \( g \) (b) and \( 4\pi r^2 P \) as a function of distance \( r \) from the solute were computed from microscopic Gauss’s law without explicit solvent (red line), macroscopic Gauss’s law (blue line), and MD simulations (black line).

The performance of calculating \( g(r) \) and \( P(r) \) using microscopic Gauss’s law. The \( g \) and \( P \) from MD simulations were compared with those obtained from microscopic Gauss’s law. The results show that the solution from microscopic Gauss’s law can yield the near-solute water structure (Figure 4). Both \( g \) and \( 4\pi r^2 P \) behave distance solute oscillation decay as observed from MD simulation.

**Conclusions**

Gauss’s law, Ampere’s law, and Faraday’s law govern the electromagnetic interactions between charged molecules in vacuum. Maxwell treated the polarized/magnetized molecules as dielectric continuum, and the derived equations govern the electromagnetic interactions between macroscopic charged objects in materials. Nevertheless, the near-solute dielectric polarization from Maxwell’s equations was inconsistent with observed from MD simulations. Hence, the equations were derived herein that can deal with electromagnetic and vdW interactions between molecular solutes in a macroscopic system containing Avogadro’s number of solvent molecules. With the rapid development of nanotechnology, concerning about electromagnetic radiation effects to humans, and the inefficiency/inadequacy of current methods to study time-dependent electromagnetic interaction between molecular solutes in a macroscopic system, the strategy presented herein to derive microscopic electrodynamics equations appears timely and fills an important gap.

**Acknowledgements**

The author gratefully acknowledges the support provided by Carmay Lim.
References

Opportunities from NSC

• **Call for applications—“Initiative Research Cooperation among Top Universities between UK and Taiwan”**
  2. Deadline for proposal: June 15, 2012

• **2013 NSC-DAAD Joint Research Cooperation**
  2. Deadline for proposal: June 15, 2012

• **2013 NSC-GACR Joint Research Cooperation**
  2. Deadline for proposal: June 21, 2012

• **2013 NSC-SAS Joint Research Cooperation**