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STOPPING MODEL OF ELECTRON IN METAL BASED ON QUANTUM MECHANICS

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ABSTRACT

With the improvement of computing capacity of computers, it is possible to broaden new horizon in classical physics and use new models in analogue simulation. Recently, it is possible that the detailed process of discussing energy exchange between metal ion and electron in simulation of quantum mechanics: low-energy electron radiation damage cascade can be simulated by directly using the tight coupling method of time dependence, and ion heat transmission with rapid movement in hundreds of atomic system can be calculated by using time domain density functional theory (TDDFT). These simulations do not evenly influenced by simplified approximate linear and electron, so a new electronic stopping model can be added in some certain level. This paper started from quantum mechanics explaining the basis of particle movement in atom, respectively discussed the frictional drag in the process of the electron motion, and the distribution of electron temperature model; finally, came to some meaningful conclusions by simulating the particle movement through respectively using the Ehrenfest Model, new model, Tocarlo and Victoria Model with a simple viscous drag and density dependence (marked as Model C-V).

Keywords: *Quantum mechanics, Electron Motion, TDDFT, Ehrenfest Model, Model C-V; Metal Electron Stopping*

1. INTRODUCTION

The difference between metal and insulator lies in their electron density of Fermi level, a large number of free electron exists in metal that can be stimulated in lower energy state. When metal is in equilibrium, there is a little energy exchange between electron and ion, or the there is a small fluxion of ion energy in between. And because thermal energy kT is usually less than Fermi energy E_F, the system of electron energy in metal is still approximates the electric energy of ground, Oppenheimer separation model is used in metal. But when ion and electron system are out of equilibrium, the energy exchange between them appears very important, high energy ion, such as radiation damage, electronic sputtering, ion channel, etc delivers a large portion to low energy electron gas, this process is called electronic stop[1]. By contrast, ion which loses energy of excitation electron in current carrying conductor will produce electric current.

Recently, molecular dynamics (MD) simulated radiation damage cascade showed that electronic stopping can promote or restrain the production of material defects in the productive process, this mainly depended on strength of coupling of ion and electron. When the strength of coupling of ion-electron increased from zero, in cooling stage, ion transmitted energy to electron, thus leading to the overflow of electron, so in the process of quenching, defects existed in material from beginning to end. When the strength of coupling was high enough, the heating speed of electronic system is much faster than the heat that electron can take away, then electron served as a heat reservoir, annealing of defects were allowed. The simulation of sputtering showed that electron heating can lead to a hot surface form concentrating effect, influence intensively the formation of secondary ion.

In a standard electronic parking chart, ion moved equably in electron gas. Electron replied this moving ion with a limited time, electron cloud lags behind the ion movement at the same time, produced coulomb force which hauled back ion and made its speed slowly[2]. Ion energy transfered to electron, and gave dielectric function relatives to the frequency of the first order imaginary part, it was called electronic damage function. Lindard research in 1954 thought that this electronic model was limited in low speed,

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electron can provide a viscous drag to limit proportion and anti-parallel of a moving electron.

But this kind of physical model was out of standard medical image, it depended on all instantaneous position of atom on the track. Of course, in the reality, behindhand electron current ion induction movement enhanced some restraints to weaken other electronic movements, thus leading to the decrease of interior speed. This paper applied chemical methods to realize electronic stopping and illustrated the reason of they were much better than molecular dynamics model of electronic effect.

2. THE EXPLANATION OF QUANTUM MECHANICS IN PARTICLE MOVEMENT

The coupling between a intact theory explanation ion and electron needs to use two electrons and phonon described by quantum mechanics. But the calculation is too cumbersome base on this theory, few atom can be used directly to carry on dynamic simulation[3]. What is luckily is that when energy transfers from high ion to low electron, a so-called Elon Dynamics model can be used precisely to describe. In this kind of method, these ions are regarded as classical point like particle, like electron dynamic model, but experience depends on the instantaneous state of electronic movement, this can solved by using Schrodinger's time-varying equation.

The quantitative model of electronic stopping is based on time domain density functional theory (TDDFT), it is completely suitable under some limit conditions, but it can not be used in electron dynamic step[4]. If the energy between tracks is too large, the affected areas will enlarge quickly and the simulation model will also enlarge; but when the energy between tracks in small, independent energy will transfer from ion to electron, and can produce energy spectrum density of electronic excitation (from meV to keV) which is very narrow.

Here considered a classical atomic theory, assume M only represents quality. The position of atom is represented by three-dimensional vector $\vec{R}$ and their three-dimensional momentum vector $\vec{P}$, and electron wave function and their state function can be represented by single particle density function[5]:

$$\hat{\rho}(t) = \sum_i f_i \left|\phi_i(t)\right\rangle\left\langle\phi_i(t)\right| \quad (1)$$

f_i --the track of wave function;

$\phi_i(t)$ --the wave function of single particle;

t --time.

The initial position of particle track set at the moment $t = 0$ and initial temperature moment, but still remain stable in simulation, wave function $\phi_i(t)$ can confirm potential atomic movement according to time domain Schrodinger equation. In coupling system, Energy can be wrote as [6]

$$E = \frac{\left|\vec{P}\right|^2}{2M} + U(\vec{R}) + Tr(\hat{\rho}\hat{H}(\vec{R})) \quad (2)$$

E ——Ehrenfest Energy;

$U(\vec{R})$ -- repulsive force between ions;

$\hat{H}$ --Hamilton binding force.

Equation of motion of Ehrenfest method[7,8]:

$$\frac{d\vec{R}}{dt} = \frac{\vec{P}}{M} \quad (3)$$

$$\frac{d\vec{P}}{dt} = -\Delta_{\vec{R}} U(\vec{R}) - Tr(\hat{\rho}\nabla_{\vec{R}}\hat{H}) \quad (4)$$

$$\frac{d\hat{\rho}}{dt} = \frac{\partial\hat{\rho}}{\partial t} = \frac{1}{ih}\left[\hat{H},\hat{\rho}\right] \quad (5)$$

In these three equations, that is quantum-mechanical Liouville formula which describes the evolution situation of its energy density with the set ion wave function changes over time according to time domain schrodinger's equation. Now, according to classical atomic model, applied Hamilton Theory at the same time, build up a mathematical model of electron evolution situation based on quantum mechanics, ion contents with Newtonian dynamics.

3. THE ELECTRONIC FRICTION IN MOLECULAR DYNAMICS(MD)

As the figure1 shows, in a mass of low energy tracks, the energy transfer between ion and electron could carry on along with a integral track[9]:

$$\Delta E_{model}(t) = \int_0^t \sum_a \beta_a(\vec{R}(\tau))\left|\vec{V_a}(\tau)\right|^2 d\tau \quad (6)$$

Here can compared with Ehrefest energy transfer formula[10]

$$\Delta E_{Ehr}(t) = Tr(\hat{H}(\vec{R}(t))\hat{\rho}(t)) - Tr(\hat{H}(\vec{R}(t))\hat{\rho}_0(\vec{R}(t))) \quad (7)$$

$\hat{\rho}_0(\vec{R})$ -- electron density stable operator.

These two indexes of energy transfer can use standard linear regression compared with assessment quality suitable empirical model. For low electronic temperature, the transfer energy rate of single electron is extremely high, when increase environment dependence （ Caro & Victoria),

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further increase this effect, as figure2 shows. It is not supported in low energy transfer, this is because the kinematic velocity of particle is lower in low energy transfer, the result is not obvious consequently.

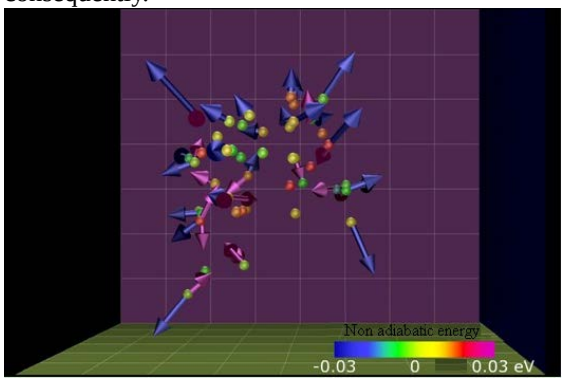

Figure 1: 30 Frame Per Second Photographed Locus In The Process Of Ehrenfest Dynamics Simulation

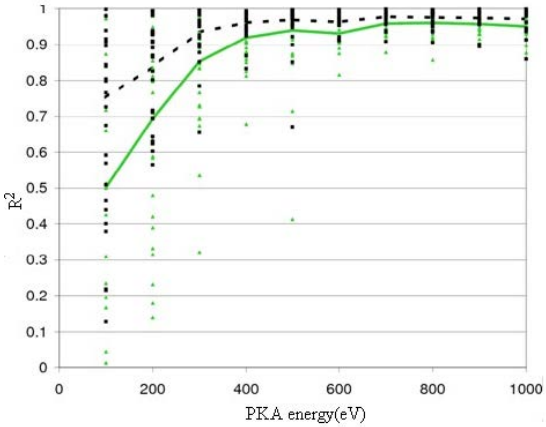

Figure 2: Value R^2 Of Energy Step In Damping Model

Embedded or extensible codec in the laminar organization of the bit stream, from the top to independent decoding.The first floor, the so-called core layer, included a necessary data, it synthesized the effective data of a minimum quality and bandwidth. The topmost layer is called to strengthen a layer, it is the bandwidth used to raise product quality and signal. According to the network discharge, the decoding machine can adapt to compare to lead especially of top and bottom motion, this is very beneficial to the data that provides a core layer. In addition, compare especially the rate own the ability of suitable terminal. The end can expand to code after the customer can pay, the customer gets into an interview then and very easily and gets the multimedia of owning the tallest quality.

Embedded coding, speech and audio coding technology has caused extensive attention. Because sample frequency and ratio lead especially of increment, transformation coding while postponing technique up have very great advantage, predict a coding technique such as the line. The transformation coding involves quantity to turn of repeatedly transformation, usually exist the having of frequency transformation FFT, DCT, microwave transformation or MDCT in time. Exist many coding techniques now, they can deliver coefficient, the simplest technique is to measure each coefficient mark quantity to turn. Amount of vector's turning may gain advantage more, but increase complexity in this aspect[11].More complicated method, turn such as the spheroid amount of vector or the quantity turn the amount of mark of vector coding, the ratio allowed especially rate significant decrease. Turn a coefficient method according to the quantity, use transformation coding on a coder that can expand coding, mean a very wise way. Embedded bit stream coefficients were compared, quantization coefficient method should be able to detect more and more close to the original bit rate value.

In addition, compare lose the process at spreading especially in, the most important coefficient usually is the biggest, and first deliver. Be worth from these, the coder reaches agreement a code machine can from most show the wave band of Zhao to compute a ratio allotment especially[12].However, to should alls of a coding need to rebuild coefficient, the not complete coding will be thrown , because they can not help to rebuild coefficient. Consequently want in consideration of each , the flat surface may suit more than coding especially.

Such as embedded microwave or set of hierarchical tree algorithm can achieve this point size. The initial research of still images, i.e. 2 dimensional signal progressive transmission, can also be used for audio coding. Through organized into a tree transformation coefficient, transmission of embedded bit stream, wherein the first represented is the most important factor is the most important, then encodes a smaller coefficient, the last transmission is the most important factor. However, the resulting expansion, may with the increasing coefficients are simple communication, lead to errors. This paper presents a kind of algebraic transform coefficient quantization method. In a framework based on coefficient, are gathered here band. Included in each band is a factor, the correlation coefficient can be detected.

4. ELECTRONIC TEMPERATURE

Ehrenfest model can provide any mechanism to

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make both electron and ion balanced, so the end simulation of electronic energy distribution does not need heating simulation[13]. However, in the actual process, atomic movement produces a large number of very small electronic energy transfer, thus leading to electronic energy proceeds energy exchange in entire three-dimensional space. Therefore, if the initial electronic temperature is zero, all tracks are occupied by electron which is below Fermi level, all tracks that are higher than Fermi level are empty, this distribution pattern accords with classical distribution pattern. Chart1 gives various kinds of distribution pattern.

Table 1: Distribution Model Of Density Function

Distribution model	Failure density function	Reliability model
Weibull distribution	$\beta\vec{V}$	$\beta\vec{V}$
Exponential distribution	$\beta\vec{V}$	$\beta\vec{V}$
Normal distribution	$\beta\vec{V}$	$\beta\vec{V}$
Logarithm normal distribution	$\beta\vec{V}$	$\beta\vec{V}$

5. DIRECTIVE FORCE

As discussed above, electronic friction is that a viscous damping-- $\beta\vec{V}$ is usually added in molecular dynamics simulation(MD). Physical experiment experience and the result of Ehrenfest simulation show that this practice is feasible in some certain degree, but β is not a scalar constant surely. Firstly, just as the research of Caro & Victoria showed that the size of damping is the function of local electronic density; Secondly, under very high electronic temperature, there is only emission of phonon, but few absorption, ion proceeds Brownian movement affected by acting force of electron, but damping is not certain; Thirdly, if all atoms move in uniform velocity, then there is no damping between electron and ion, so, the value of β depends on relative speed, rather than absolute speed; Fourthly, if energy among atoms is enough, it would promote electron move from low level to high level, thus making energy band structure remain stable; Fifthly, moving electron produced by electron excitation could accumulate as time goes on, so damping possesses historical dependence; Finally, electron excitation could lead to strengthen a part and weaken an other part, so nonadiabatic electronic force depends on its direction and properties. Conclusion: β is a tensor, it depends on all ions and its historical position and relative speed.

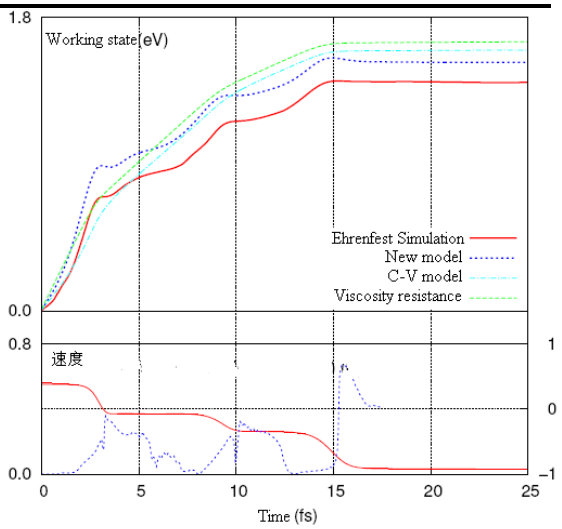

Figure 3: The Result Of Nonadiabatic Energy Analogue Simulation

Algebraic quantization is actually very simple, because it is equivalent to a sorting algorithm, i.e. in a band, the coefficient values according to the order of arranging. In the following, we use audio coding experiments to prove, algebraic quantization is easy to be applied.

Algebraic quantization has been used for multimedia digital signal coder. This kind of breadth took the speech plait decoding machine to provide a built-in ratio to flow especially, can 8-32 k bits/s ratio especially rate the decoding decode in the machine at 10 ms the plait of. The structure of this coder constitutes to from three layers. First, an abruption can take structure to separate a part of a part of the low wave band(LB) and high wave band(HB);The core layer is a part that codes to input a low wave band of signal. This of ITU- T the coder of the G.729 use a 8 kits/s ratio especially rate, the first floor depends on a microwave filter and makes use of a bandwidth to

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expand a technique, as a result have an additional 2 kits/s ratio lead especially;WPD of the to build up layer of end provided 14 WPS that will send outwash according to the 10 kbits/s energy(the bandwidth of G.729 expands) according to gradually decrease in proper order transmission. Flap to pass 16 class the not- even mark measure of the quantity turn a machine to attain quantity to turn.

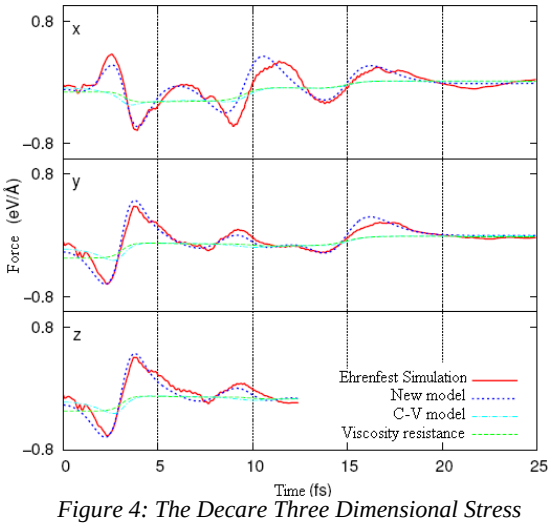

Figure 4: The Decare Three Dimensional Stress Situation In The Process Of Nonadiabatic Simulation

The above panel in figure3 shows that Ehrenfest simulation in collision cascade of main chaining atom nonadiabatic force. Under this kind of situation, the moving atom moves along its path, it meets the first atom and experiences a oblique collision. The under panel shows that the speed of ion(active line), and the included angle cosine of its speed and non-adiabatic force in Ehrenfest simulation (as figure shows that the speed is appreciable).

Figure 4 shows that three dimension non-adiabatic force in Decare reference frame. It proceeded a simulation by respectively using Ehrenfest model, new model, a simple viscous drag and density dependent Carlo&Victoria model (marked as C-V model)

6. CONCLUSION

The simulation of quantum mechanics shows that on the basis of electron friction thought described electronic prevent success and convenience provides the model device of average power from ion subsystem transfer. A simple viscous damping coefficient is applied in this model, it can provide enough modeling of energy transfer rate, and make damping coefficient depend on electronic density and calculate transitionally probable precision among specific stripes that can be increased. The approximate form which is suitable in MD simulation is put forward at the same time, studies the directional properties of electron heating nonadiabatic force. This is a model calculation with little extra calculating cost compared with previous calculations.

In the next several years, the application of simple Halmiton model is expected to use in time domain density function theory(TDDFT), and also provide accurate estimating stopping parameters in the meantime, and applies in the prediction of molecular dynamics simulation. The current theories that is the theory of electron heat transport and autonomous stimulation are more difficult to become actual method of simulation, but it is still making progress. The quantum simulation of energy transport and exchange between ion and electron in metal could come true in a few years.

REFERENCES:

[1] Y. Tana, M. Sata, “Asymmetric fingerprinting based on 1-out-of-n oblivious transfer”, Proceedings of International Conference on Computer Application in multimedia, IEEE Conference Publishing Services, February 25-28, 2010, pp. 622-632.

[2] Y. Tana, M. Sata, “Asymmetric fingerprinting based on 1-out-of-n oblivious transfer”, *IEEE Communications Letters*, Vol. 14, No. 5, 2010, pp. 101-111.

[1] Gao, F., Bacon, D.J., Flewitt, P.E.J., and Lewis, T.A., The electron-phonon coupling on defect production by displacement cascades in alpha-iron, Modeling and Simulation in Materials Science and Engineering, Vol. 556, No. 6, 2008, pp. 727-734.

[2] Kapinos, V.G., and Bacon, D.G., “Inuence of ion-electron interaction on the formation mechanism of depleted zones in displacement cascades in metals”, *Phys. Rev. B*, Vol. 50, No. 13, 2011, pp. 194-205.

[3] Nordlund, K., Wei, L., Zhong, Y., and Averback. R.S., “Role of electron coupling on collision cascade development in Ni, Pd, and Pt”, *Phys. Rev. B*, Vol. 57, No. 13, 2008, pp. 965-977.

[4] Duvenbeck, A., andWucher, A., “Low-energy electronic excitation in atomic collision cascades: A nonlinear transport model”, *Phys. Rev. B*, Vol. 72, No. 16, 2010, pp. 5408-5417.

ISSN: 1992-8645 www.jatit.org E-ISSN: 1817-3195

[5] Duvenbeck, A., Weingart, O., Buss, V., and Wucher, A., "Electron promotion and electronic friction in atomic collision cascades", *New J. Phys.*, Vol. 9, No. 38, 2007, pp. 46-55.

[6] Race, C.P., Mason, D.R., Finnis, M.W., Foulkes, W.M.C., Horsffeld, A.P. and Sutton, A.P, "The treat- ment of electronic excitations in models of radiation damage in metals", *Rep. Prog. Phys.*,Vol. 5, No. 7, 2010, pp. 78-90.

[7] McEniry, E.J., Bowler, D.R., Dundas, D., Hors_eld, A.P, Sffanchez, C.G. and Todorov, "Dynamical simulation of inelastic quantum transport", *J. Phys.*: Condens. Matter, Vol. 19,No. 7, 2007, pp. 196-201.

[8] McEniry, E.J., "Modeling non-adiabatic processes using Correlated Electron-Ion Dynamics", *Eur. Phys. J. B*, Vol. 25, No. 5, 2010, pp. 561-570.

[9] Rutherford, A.M. and Duffy, D.M., "The effect of electron-ion interactions on radiation damage simulations", *Journal of Physics: Condensed Matter*, Vol. 496, No. 19, 2009, pp.176-184.

[10] Duffy, D.M. and Rutherford, A.M., "Including the effects of electronic stopping and electron-ion interactions in radiation damage simulations", *Journal of Physics: Condensed Matter*, Vol. 19, No. 1, 2007, pp. 556-564.

[11] Ritchie, R.H., "Interaction of charged particles with a degenerate Fermi-Dirac electron gas", *Phys. Rev.*, Vol. 114, No. 64, 2009, pp. 645-653.

[13] Le, Page, J., Mason, D.R., and Foulkes, W.M.C. "The Ehrenfest approximation for electrons coupled to a phonon system", *J. Phys.: Condens. Matter*, Vol. 5, No. 7, 2008, pp. 67-74.