EFFECTS OF Ni_3Ti (DO_{24}) PRECIPITATES AND COMPOSITION ON
Ni-BASED SUPERALLOYS USING MOLECULAR DYNAMICS METHOD

GOH KIAN HENG

UNIVERSITI TEKNOLOGI MALAYSIA

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GOH KIAN HENG

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ABSTRACT

The main aim of this study is to simulate and investigate the gamma and gamma prime phases structure stability and behaviour of misfit dislocation-precipitate with additional of Ni_3Ti (DO_{24}) in Ni-based superalloys using MD at 10 K, 293 K and 1000 K. The Ni_3Ti are homogeneously distributed through γ phase and the percentages are varied from 0.22%, 0.5%, 0.89% and 2.11%. MD is capable to produce three dimensions modelling based on time evolution of a set of interacting atoms and integrating their equation of motion. The Embedded Atom Method (EAM) is used to calculate phase stability, point defect properties, surface energies and relaxation for Ni-Ti-Al system. The empirical embedding energy function, electron density function and interatomic pair potential function used by this method are obtained. The conclusion of this simulation shows that distribution of Ni_3Ti is vital in determining the Ni-Ni_3Al phase stability. The data of temperature, total energy, stress in x-axis, stress in y-axis, stress in z-axis and volume are plotted and snapshot of each percentage of Ni_3Ti added is taken at different step. At higher temperature (1000 K), it is more favourable and stable condition for higher Ti concentration (9L 2.11%) because of lower energy level and more stable temperature condition.

ABSTRAK

Tujuan utama kajian ini adalah untuk menjalankan proses simulasi bagi menyiasat kestabilan fasa dan ketidakpadanan struktur gamma dan gamma prime serta kehelan-mendakan dengan penambahan Ni_3Ti (DO_{24}) dalam superalloys berasaskan Nickel menggunakan Molecular Dynamic (MD) pada 10 K, 293 K and 1000 K. Ni_3Ti diedarkan secara serata melalui fasa γ dengan peratusan penambahan Ni_3Ti diubah dari 0.22%, 0.5%, 0.89% and 2.11%. MD berupaya untuk menghasilkan pemodelan 3 dimensi yang berdasarkan evolusi masa satu set atom yang berinteraksi sesama sendiri dan mengintegrasikan persamaan pergerakan yang terlibat. Embedded Atom Method (EAM) digunakan untuk mengira kestabilan fasa, ciri-ciri kecacatan titik, tenaga permukaan dan kelonggaran untuk sistem Ni-Ti-Al. Fungsi tenaga pembenaman empirikal, fungsi ketumpatan elektron dan fungsi potensi pasangan atom yang digunakan melalui kaedah ini, dapat diperolehi. Kesimpulannya, hasil daripada proses simulasi ini menunjukkan bahawa pembahagian Ni_3Ti adalah sangat penting dalam menentukan kestabilan fasa Ni-Ni_3Al. Data suhu, jumlah tenaga, tekanan di x-paksi, tekanan di paksi-y, tekanan di paksi-z dan isipadu diplotkan dan gambar setiap peratusan Ni_3Ti diambil pada langkah yang berbeza. Pada suhu yang lebih tinggi (1000 K), keadaan ada lebih sesuai dan stabil bagi peratusan Ti yang lebih tinggi (9L 2.11%) kerana jumlah tenaga ada lebih rendah dan keadaan suhu yang lebih stabil.

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LIST OF SYMBOLS

γ	-	Gamma phase (Ni)
γ'	-	Gamma prime phase (NI_3Al)
TEM	-	Transmission Electron Microscopy
Ni	-	Nickel
Ti	-	Titanium
Al	-	Aluminium
MD	-	Molecular Dynamic
Ni_3Al	-	Nickel Aluminide
Ni_3Ti	-	Nickel Titanide
F^α	-	Force acting on atom α
t	-	Time
m^α	-	Mass vector position of atom α
r^α	-	position vector position of atom α
E_{tot}	-	Total potential Energy
Δt	-	Time difference
$r^{\alpha\beta}$	-	Scalar distance
$\emptyset$	-	Pair wise interaction between atoms
$F(\bar\rho)$	-	Embedding function
$\bar\rho_\alpha$	-	Density at atom α
t_α	-	Types of atoms α
t_β	-	Types of atoms β
g	-	Linear transformation parameter
s	-	Scaling transformation parameter
$\rho(r)$	-	Density function
β	-	Adjustable parameter for density function
$\emptyset(r)$	-	Pair wise interaction function
D_M	-	Depth at the minimum of the energy curve

R_M	-	,Position of the minimum at the minimum of the energy curve
α_M	-	Curvature at the minimum of the energy curve
Å	-	Angstrom
eV	-	Electron Volt
K	-	Kinetic Energy
m^α	-	Mass of atom α
v^α	-	Velocity of atom α
k_B	-	Boltzmann constant
N	-	Total number of atoms in the system
T	-	Instantaneous temperature
T_C	-	Constant temperature
K	-	Kelvin
σ	-	Stress
V	-	Volume
FCC	-	Face Centred Cubic
HCP	-	Hexagonal Closed Packed
CNA	-	Common Neighbour Analysis
EAM	-	Embedded Atom Method

CHAPTER 1

INTRODUCTION

1.1   Introduction

In the recent past, with the rapid development of the computer technology, molecular dynamics (MD) simulation based on the computer simulation has played more and more important role in understanding the mechanical properties of materials. Computer simulation provides a direct route from the microscopic details of a system to macroscopic properties of experimental interest [1].

Nickel based superalloys have combination of high temperature strength, toughness, and resistance to degradation in corrosive or oxidizing environments. These materials are widely used in aircraft and power-generation turbines, rocket engines, and other challenging environments, including nuclear power and chemical processing plants.

Ni-based superalloys consist of a high volume fraction of cuboidal γ' phase (L12 structure) separated by narrow γ channels (FCC solid solution) [2]. The γ´ cuboidals generally align along [100] lattice direction, each of which as an average edge length of the order 500nm. Due to the edge length of the γ' cuboidal is very small, there is a vast interfacial region between the solid solution γ phase and the ordered γ' precipitates [3]. It is believed that the structure and properties of γ/γ' interface greatly affect the shape,

the size and coarsening rate of γ' precipitate, which in turn is a major factor influencing creep rupture strength of superalloys [4].

Since the lattice parameters of the two phases are similar but not identical, a stress field resulting from the lattice mismatch will be created. This will lead to the unstable stress field at the interface. In order to minimize the elastic stress field between the γ and γ' phase, the atoms on the interface will rearrange themselves. This justified with the principle of minimum energy. This stage is known as the self-accommodating process. Gradually, the misfit dislocations will be created in the interface to reduce the distorted energy. A plastic deformation is formed due to the misfit dislocation move in the interface cause permanent change of shape [5].

1.2   Background of Study

Computer simulation for example molecular dynamics has been used for studying mechanical properties of nickel based superalloys for last few ten years. The nickel based superalloys have been used widely in industry application. Nucleation of a single defect on the atomic scale sometimes brings about fatal malfunction of such devices. Therefore, it becomes important to understand the mechanics and mechanism of defect nucleation on a microscopic scale. Although the fracture of materials has been investigated for many years, there remain many uncertainties with regard to the nucleation process because of experimental difficulties.

In microelectromechanical systems (MEMS), thin films of Ni and Ni alloy have been widely used. As the dimensions of components in these systems decrease to the micro-scale, even the nano-scale, the interfacial phenomena significantly differ to the counterparts on the macro-scale. A better understanding of micro- or nano-tribology will benefit the fabrication of the small components. Thus, molecular dynamics simulations have been conducted to investigate the nanoscratch behaviour of nickel [6].

The recent rapid progress of computers makes the microscopic simulation of solid structures possible. Cyclic stress–strain curves and fatigue crack growth can be investigated by molecular dynamics. Nanoscale fatigue damage simulations were performed in nickel single crystals[7]. The mechanical properties of nickel nanowire at different temperatures are studied using molecular dynamics simulations [8].

Besides that, the effects of nickel coating on the torsional behaviours of single-walled carbon nanotubes (SWCNTs) subject to torsion motion are investigated using the molecular dynamics simulation method [9]. Extremely high strain rate effect on the mechanical properties of nickel nanowires with different cross-sectional sizes is investigated by Dan Huang et al. The stress–strain curves of nickel nanowires at different strain rates subjected to uniaxial tension are simulated [10].

T.W. Stone also conducted molecular dynamics simulations using the embedded atom method potentials to describe the interparticle behaviour of two single crystal spherical nickel nanoparticles during compaction based on the particle size and contact angle [11].

The mechanism of dislocation at the γ/γ' interface of Ni-based superalloys, for example; the misfit dislocation, dislocation pinning by γ'-precipitates and the nucleation of super dislocation in precipitates, is of great interest in understanding the mechanical performances of the superalloys. Several studies have been made on the phenomena at the interface, with both experiment and analytical approaches, for instances direct observation of dislocation behaviour by high resolution TEM and finite-element analysis based on geometrically necessary dislocation theory [12].

Aihara et al. have conducted a molecular dynamics study on the strength of a γ/γ' interface that idealizes a $\gamma/$ γ' interface in Ni-based superalloys. The simulation is conducted on a nanoscopic wire with a laminate structure made from staked γ (Ni) and γ' (Ni_3Al) layers, so that the effect of the free surfaces is significant and thus the

dislocation behaviour in the simulation may not be consistent with that in the bulk of the γ/γ' microstructure. Moreover, it seems of greater interest to investigate the dislocation behaviour not only at a planar interface but also at multiple intersections of interfaces such as an apex or edge of the cuboidal precipitate [12].

Therefore, the effect of alloying element especially the DO_{24} Ni_3Ti added to Ni-based superalloys are great interest to investigate the behaviour of misfit dislocation in γ/γ' interface because it is still new and can be explored.

1.3 Problem Statement

The interactions between these γ and γ' phases affect the properties of Ni-based single-crystal superalloys. Capability in understanding the microscopic structure of the γ and γ' phases are of the utmost importance in the development of novel alloys with superior mechanical properties.

Previous study has been done in order to investigate the preferential site in Ni_3Al lattices. The knowledge about the preferential site for alloying elements is useful in clarifying the role of ternary system additions in controlling the mechanical properties of Ni-based superalloys. MD simulations have been used to simulate the stability of Ni-Ni_3Al phases, interface and dislocation-precipitate interaction. However, the interaction of DO_{24} Ni_3Ti with Ni phase on atomistic scale in Ni-based superalloys is still unclear.

The stability of the Ni-Ni_3Al phases and interface are evaluated by gradually changing the alloying element (DO_{24} Ni_3Ti) concentration in either Ni phase. The energy and semi-coherent interface between Ni and Ni_3Al phases are also investigated by changing the combination of crystal orientation. Addition of alloying element (DO_{24} Ni_3Ti) will lead to higher melting point and hardening coefficient.

1.4   Objective of Study

The main objective of this study is to simulate and investigate the effects of Ni_3Ti with DO_{24} structure precipitate and composition on Ni-based superalloys using molecular dynamics method.

1.5   Scope of Work

The scope of work is clearly define the specific field of the research and ensure that the entire content of this project is confined the scope. This project is done base on the scope below:

1. Study the effect of alloying element-DO_{24} Ni_3Ti in Nickel Based Superalloys.
2. Utilize Molecular Dynamic (MD) method.
3. Learn the programming language – Fortran 90.
4. Analyze and develop existing MD coding.
5. Alter the additional percentages and distribution.
6. Study the changes in the simulation cell.

1.6   Significance of Study

This project has several important outcomes which included as the following;

i.   Comparison for analytical and experiment's result with computer simulation's result.

ii.   Improve the understanding and gain new knowledge for adding alloying element (DO_{24} Ni_3Ti) and varies the percentages of additional element in Ni-based superalloys.

iii.   New milestone to explore new area of study of atomic computer simulation in Mechanical Engineering Faculty (FKM), UTM.

REFERENCES

1. Yan Jia, Heng Liu, Lie Yu.(2009). *Propagation of Stress Wave in Nickel Single Crystals Nanofilm via Molecular Dynamics*, International Conference on Automation and Logistics, pp.1396-1400

2. Nabarro F R N and Villiers H L.(1995). *The physics of Creep* (London: Taylor & Francis)

3. Anton D L in: Westbrook J H and Fleisher R Leds.(1994). *Intermetallic Compounds* (New York: Wiley) 2, 3.

4. Mirkin I L and Kancheev O D(1967) Met.Sci. *Heat Treat*. 1-2, 10.

5. Hong-Xian Xie, Chong-Yu Wang and Tao Yu. (2009). *Motion of Misfit Dislocation in an Ni/Ni₃Al Interface: A Molecular Dynamics Simulations Study.* China: Central Iron and Steel Research Institute, Beijing.

6. Y.Gao,C.Lu, N.N. Huynh, G. Michal, H.T. Zhu, A.K. Tieu, (2009). *Molecular dynamics simulation of effect of indenter shape on nanoscratch of Ni*, Wear, 267, pp. 1998–2002.

7. G.P. Potirnichea, M.F. Horstemeyer, B. Jelineka, G.J. Wagner, (2005). *Fatigue damage in nickel and copper single crystals at nanoscale, International Journal of Fatigue*, 27, pp. 1179–1185.

8. A.R. Setoodeh, H. Attariani, M. Khosrownejad, (2008). *Nickel nanowires under uniaxial loads: A molecular dynamics simulation study*, Computational Materials Science, 44, pp.378–384.

9. Hai Yang Song, Xin Wei Zha.(2011). *Molecular dynamics study of effects of nickel coating on torsional behaviour of single-walled carbon nanotube*, Physica B, 406, pp. 992–995.

10. Dan Huang, Qing Zhang, Pizhong Qiao.(2011). *Molecular dynamics evaluation of strain rate and size effects on mechanical properties of FCC nickel nanowires*, Computational Materials Science, 50, pp.903–910.

11. T.W. Stone, M.F. Horstemeyer, Y. Hammi, P.M. Gullett.(2008). *Contact and friction of single crystal nickel nanoparticles using molecular dynamics, Acta Materialia*, 56, pp.3577–3584.

12. Kisaragi Yashiro, Masato Naito, and Yoshihiro Tomita. *Molecular Dynamic Simulation of Dislocation Nucleation and Motion at γ/γ' interface in Ni-based Superalloys*. Kobe, Japan: Department of Mechanical Engineering, Faculty of Engineering, Kobe University, Rokkodai, Nada.

13. Michael P. Allen,(2004). I*ntroduction to Molecular Dynamics Simulation*, NIC Series, Vol. 23, ISBN 3-00-012641-4, pp. 1-28.

14. Tresa M. Pollock, (2006). *Nickel-Based Superalloys for Advanced Turbine Engines: Chemistry, Microstructure, and Properties*, Journal of Propulsion and Power, Vol. 22, No. 2, pp.361-374.

15. Yong Cao, Jingchuan Zhu, Yong Liu, Zhonghong Lai, Zhisheng Nong.(2013). *First principles studies of the structural, elastic, electronic and thermal properties of γ´-Ni₃Ti*, Physica B, 412, pp.45–49.

16. M.M. Verdian, K. Raeissi, M. Salehi, S. Sabooni,(2011). *Characterization and corrosion behaviour of NiTieTi2NieNi3Ti multiphase intermetallics produced by vacuum sintering*, Vacuum, 86, pp.91-95.

17. K. Hagihara, T. Nakano, Y. Umakoshi,(2003). *Plastic deformation behaviour in Ni3Ti single crystals with D024 structure*, Acta Materialia, 51, pp.2623–2637.

18. J.X. Zhang , J.C. Wang, H. Harada, Y. Koizumi,(2005). *The effect of lattice misfit on the dislocation motion in superalloys during high-temperature low-stress creep*, Acta Materialia, 53, pp. 4623-4633.

19. Joy RP Djuansjah, Kisaragi Yashiro and Yoshihiro Tomita, (2008). *Computational Study on Misfit Dislocation in Ni-Based Superalloys by Quasicontinuum Method*, Materials Transactions, Vol. 49, No. 11, pp. 2507- 2514.

20. Dr Billy D. Todd. *Introduction to Molecular Dynamics, Centre for Molecular Simulation*, Swinburne University of Technology.

21. D Farkas, D Roqueta, A Vilette, and K Ternes. (1996). *Atomic Simulation in Ternary Ni-Ti-Al- Alloys.* USA: Department of Material Science and Engineering, Virginia Polytechnic Institute, Blacksburg.

22. Voter and Shao Ping Chen. (1987). *Accurate Interatomic Potentials for Ni, Al and Ni₃A.* Los Alamos: Theoretical Division, Los Alamos National Library.

23. D Farkas. (1994). *Interatomic Potential for Ti-Al with and without Angular Forces*. USA: Department of Material Science and Engineering, Virginia Polytechnic Institute, Blacksburg.

24. Wong Chin Chun. (2012). *Molecular Dynamic Simulation of Titanium Addition in Ni-Based Superalloys*. Faculty of Mechanical Engineering, Universiti Teknologi Malaysia.