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Molecular dynamics simulation of stress field around edge dislocations in Aluminum

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ABSTRACT

Selection of potential functions is a very important step in molecular dynamics (MD) simulations due to its effects of the preciseness and reliability of the simulations. Different potential functions have been developed for atomistic simulations of materials and the embedded atom method (EAM) can be considered as the most successful class of potential function with acceptable accuracy and performance. Reliability of a potential function is determined by comparing simulation results with basic experimental results or physical and mechanical models. In the current work, the calculated stress tensor around an edge dislocation, based on the isotropic and anisotropic continuum models, was chosen as the basis for evaluations of some notable EAM potential functions developed for Aluminum. Qualitative and quantitative comparisons between the results of MD simulation with four selected potential functions and the continuum models were made. Every component of the stress tensor was studied separately and the potential functions were ranked according to their accuracy and the appropriate potential function was introduced. These findings can be considered as a basis for simulation of the different aspects of mechanical behavior of metallic materials.

1. Introduction

One of the important aspects of the dislocation theory is stress field around dislocations, which determines the interaction of dislocations with other defects. The stress tensor around a dislocation can be calculated based on the isotropic and anisotropic continuum models. However, for modeling the mechanical behavior of materials and relating the proposed mechanical theory to experimental observations, a more powerful technique is required. Atomistic simulations can be used as a reasonably accurate and reliable method for studying dislocation phenomena. Among various methods of atomistic simulations, molecular dynamics (MD) is an acceptable method due to its ability to give insightful vision of phenomena at the atomic level [1].

Selecting a proper potential function is a very important part of atomistic simulations' programming. Potential functions determine forces and energy of atoms throughout the simulation [2–4]. These functions are developed to match some certain material properties as accurately as possible. For example, in the study of mechanical behavior of materials, stacking fault energy, elastic modulus, shear modulus, bulk modulus and stress field around a dislocation core need to be accurate. An interatomic potential function defines interaction energy between atoms based on the physical nature of atomic bonding. Different interatomic potential functions exist and they can be classified based on the origin of formulation and values of parameters used in the functions. They can be classified into empirical, semi-empirical, and quantum mechanical ones. Both formulation and parameters of an empirical potential function is derived based on experimental results (Lennard-Jones and Morse potentials) [4,5]. In a semi-empirical potential function, the form of the function is not derived based on physical models but potential data are obtained from quantum mechanics calculations (such as tight-binding method) [4,5]. In a quantum-based potential function, all information about coordination and energy of atoms is directly produced from the solution of quantum mechanics formulation [4,5]. One of the most practical approaches for developing interatomic potential functions is the embedded atom method (EAM) [6], which belongs to the empirical class of potential functions and it might also be improved by quantum mechanics calculations. Main advantages of this class of potential functions are simplicity, acceptable accuracy and efficiency in describing large atomic systems [7]. The EAM potential functions have been growingly used for description of deformation phenomena in FCC materials that involve dislocations

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Nomenclature

a_0	lattice parameter
E_0	cohesive energy
B	bulk modulus
E	elastic modulus
G	shear modulus
v	Poisson's ratio
b	burgers vector
Ω	atomic volume
x_i	coordination vector
C_{rs}	stiffness tensor
S_{mn}	isotropic stress tensor
σ_{ij}	anisotropic stress tensor
f_K^{ij}	force vector between atoms i and j
r_m^{ij}	position vector between atoms i and j
β_{rs}^i	local stress tensor for atom i
T_{mk}	stress tensor for an atom
N	number of the nearest neighbor atoms
N^*	total number of atoms
E_v^f	vacancy formation energy
E_v^m	vacancy migration energy
γ_{SF}	stacking fault energy
γ_T	twining energy
$\gamma_s(110)$	surface energy on (110) plane
$\gamma_s(100)$	surface energy on (100) plane
$\gamma_s(111)$	surface energy on (111) plane

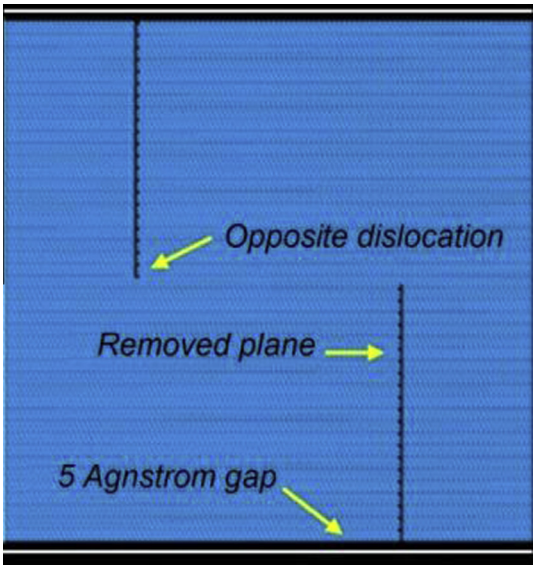

Fig. 1. The initial configuration used for the simulations.

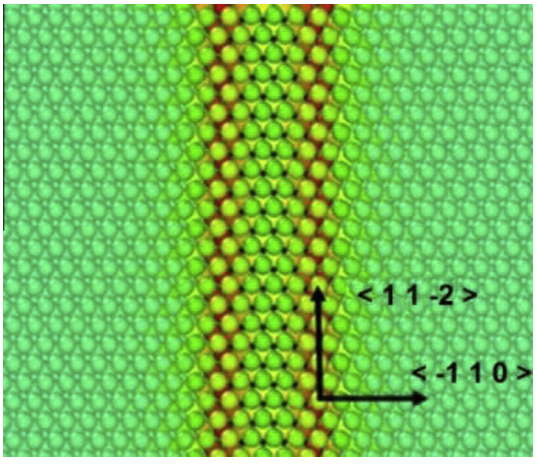

Fig. 2. Crystallographic directions of dislocation line and Burgers vector on (111) plane. Dissociated dislocation lines and stacking fault zone are clearly visible.

movement, dislocation nucleation, dissociation and interaction of dislocations [8–11].

In current work, the application of molecular dynamics technique in the study of stress field around an edge dislocation will

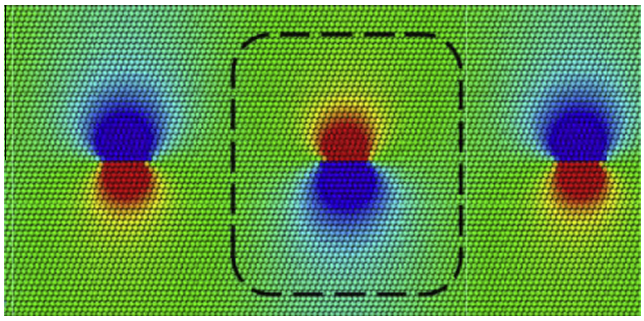

Fig. 3. The planar slice to show the effect of periodic boundary conditions and region of the simulation box used for comparisons.

Table 1
EAM potential functions used for the MD simulations and predicted properties of Aluminum.

	Experimental results [19]	Mishin et al. [16]	Zope and Mishin [17]	Liu et al. [18]	Sheng et al. [19]
Referred in this article as		P1	P2	P3	P4
a_0 (A)	4.05	4.05	4.05	4.032	4.05
E_0 (eV/atom)	−3.36	−3.36	−3.36	−3.36	−3.36
B (GPa)	76	79	79	80.9	77
C_{11} (GPa)	114	114	116.8	118	113
C_{12} (GPa)	61.9	61.6	60.1	62.3	61.6
C_{44} (GPa)	31.6	31.6	31.7	32.5	32
E_v^f (eV)	0.68	0.68	0.71	0.68	0.67
E_v^m (eV)	0.65	0.64	0.65	0.64	0.65
γ_{SF} (mJ/m^2)	120–144	146	115	128	117
γ_T (mJ/m^2)	75	76	63		62
$\gamma_s(110)$ (mJ/m^2)	980	1006	792	1105	993
$\gamma_s(100)$ (mJ/m^2)	980	943	607	1009	855
$\gamma_s(111)$ (mJ/m^2)	980	870	601	913	634
E (GPa)	70				
G (GPa)	26				
v	0.35				

Table 2
Partial dislocation distances predicted by isotropic continuum model and MD simulations with different EAM potentials.

Potential function	Simulation results (Å)	Isotropic model results (Å)
P1	12.1	7
P2	13.5	8.9
P3	14.9	8
P4	12.0	8.7