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Modeling the Stretch Behavior of the Single-Crystal Ni−Al Alloy and Its Molecular Dynamics Simulation

© Javad Alizadeh, Masoud Panjepour, Mehdi Ahmadian

Department of Materials Engineering, Isfahan University of Technology, Isfahan, Iran

E-mail: javadalizadehnoory@gmail.com

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Molecular dynamics simulation was employed in this study to investigate the atomistic mechanisms involved in the Ni−Al alloy homogeneous deformation and the mechanical properties of single-crystal Ni−Al under periodic boundary conditions (until the fracture begins). It is the objective of the present study to develop a simple mathematical model for calculating stress similar to molecular dynamics simulation while the effects of the components of the interatomic potential energy function and the different neighboring atomic shells are also determined on the total stress in the system. The model results show that the sixth nearest neighboring shell has the greatest effect on the stress−strain curve of the Ni−Al single crystal. The associated calculations in the model also show that, in the absence of the pair interaction type of the sixth nearest neighboring shell, the behavior of the material approaches a linear elastic one.

Keywords: mathematical modeling, molecular dynamics simulation, single crystal, intermetallic material