ICCES, 2023, vol.25, no.2
DOI: 10.32604/icces.2023.09968

PROCEEDINGS

Molecular Dynamics Simulations on the Pyramidal Dislocation Behaviors in Magnesium

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ABSTRACT

Magnesium is a lightweight structural metal but the industrial application is limited by its poor intrinsic ductility. Pyramidal <c+a> dislocations are believed to be responsible for the ductility enhancement whereas the dislocation plasticity of magnesium was not well studied, especially the pyramidal dislocations. In this work, molecular dynamics simulations were performed to investigate the pyramidal disloation behaviors including the decomposition of pyramidal dislocations on both pyramidal-I and pyramidal-II planes and the interactions between themselves and other dislocations in Mg. The pyramidal-I dislocations are decomposed into <c> and <a> dislocations under shear stress at 0-400K, which all reside on basal plane. At 500-700K, the dislocations are transited onto basal plane at zero stress, then decomposed into <c> and <a> dislocations under shear loading. Especially, at 700K, the dislocation is possibly decomposed spontaneously at zero stress. For the pyramidal-II dislocations, the core is glissile below 400K. At 500K, the dislocation is transited onto basal plane under shear loading. At 600-700K, basal <c+a> dislocation is formed at zero stress, but then decomposed under shear loading. Dislocation core energy is calculated to explain the observations. It is found that the energy of decomposed <c+a> dislocation is high, energy of pyramidal <c+a> dislocation is intermedium, while energy of basal <c+a> dislocation is low. In addition, systematic investigation of dislocation interactions are carried out, i.e. between <c+a> dislocations, between <a> dislocations, between <a> and <c+a> dislocations, as well as between <a> and <c> dislocations. Various new interaction products were observed and analyzed. Our results provide new insights into the behaviors of pyramidal dislocations and temperature effects.

KEYWORDS

Magnesium alloys; pyramidal <c+a> dislocations; molecular dynamics; decomposition

Funding Statement: The author(s) received no specific funding for this study.

Conflicts of Interest: The authors declare that they have no conflicts of interest to report regarding the present study.