Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E1]Poster Session 1

Symposium E

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-32]Molecular Dynamics Simulation of Crack Growth Behavior of Single Crystal γ-TiAl Alloy Under Different Nb Substitution Mode

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Because of the low plasticity at room temperature, high rate of crack propagation of TiAl alloy, its application in the aerospace has been severely restricted. The addition of Nb contributes to solving this problem.The Ti-Al-Nb ternary system has become the main trend of development of TiAl alloys, and the influence of alloying elements Nb on the properties of TiAl alloys has become the focus of extensive attention and research in the field of materials engineering.In this paper,the effect of different substitution modes of Nb on the crack propagation of γ-TiAl alloy was studied from the microscopic scale by molecular dynamics method.The effect of cracks on the performance of γ-TiAl alloys without Nb, Nb substitutional Al systems, and Nb substitutional Ti systems was analyzed.The results show that the interaction between Nb and the neighboring matrix atoms is stronger than the interaction between Ti-Al atoms before the substitution, and the doped Nb is enhanced compared to the γ-TiAl alloy without Nb. The bonding and bonding strengths between the atoms in the matrix and the atoms in the TiAl alloy increase the bond strength of the unit cell, increase the bonding force and cohesion between the surrounding atoms, and make the atoms in the crack tip region bond tightly, making it difficult to break bonds and become crack propagation. An obstacle is the passivation of the crack tip, the slower rate of crack propagation, and the change in the crack propagation path, which increases the tensile and fracture toughness of the alloy.The substitutional Ti system has a higher yield strength than the substitutional Al system, Nb occupies a sublattice of Ti, and the short-range interaction between dislocations and Nb atoms results in solid solution strengthening, which enhances the strength of the alloy.The lattice distortion of the substitutional Al system is more serious than that of the substitutional Ti system, and the dislocation density is higher and the fracture toughness is higher. The difference in this phenomenon is more pronounced at a high Nb concentration of 6%.