COMPUTER SIMULATION OF BRITTLE BEHAVIOR IN Ti_3Al

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Abstract – Orientation dependence of fracture behavior in Ti_3Al is investigated. The model of shear microcracks nucleation in basal, with screw ***a*** superdislocations coalescence, is introduced. It is demonstrated, that long-range stress of dislocations in a slip band plays an important part in the process of microcrack nucleation.

Ti_3Al (ordered hexagonal superstructure $D0_{19}$) is the main component of the number alloys, which are known as promising materials for heat-resisting and heatproof applications. Brittleness of the intermetallic compound hinders its practical applications. The orientation dependence of the fracture behaviour of a Ti_3Al single crystal was discovered as well: the deformation before fracture reaches the value of ~250% for prism slip, while for basal slip brittle fracture observes immediately after loading even with compression. The relationship between the susceptibility of a metal to cleavage and plastic relaxation of stresses near the crack tip by emitting dislocations for Ti_3Al single crystals has been studied using the Rice-Thompson model. Using the method of computer simulation the surface energy which determines the ability of a crack to opening and the energies of unstable stacking faults which determine the energies barriers that should be overcome in the processes of dislocation slip have been obtain. Criteria of brittle fracture of Ti_3Al with allowance for experimentally observed types of cleavage planes and dislocation slip systems have been estimated. Decohesion energy and the energy of unstable stacking faults for the basal plane, prismatic and pyramid planes was studied using molecular dynamic method with EAM interatomic potentials [1]. It was shown that cleavage in Ti_3Al is due to low decohesion energy values, which facilitates cracking, and high energies of unstable stacking faults, which prevents the formation of a plastic zone and stress relaxation at crack tip. An analysis of the relationship between the decohesion energy and the energy of unstable stacking faults indicates the intrinsic nature of brittleness of Ti_3Al caused by specific features of interatomic interactions in these intermetallic compounds.

The dislocation model of the formation of shear type microcracks in basal plane slip band, based at the analysis of the core structure of ***a***-superdislocations in the basal and prism planes [2,3], is discussed. It was established that and the core of the dislocations of edge as well as screw orientation in the plane of the prism is planar [4]. Nonplanar core structure of the screw dislocations in the basal plane was detected. Model for shear microcracks nucleation in basal slip band take into account the processes of coalescence of screw ***a***- superdislocations in basal plane and cross-slip into prism plane. As a result of consecutive stages of internal dislocations rearrangements the total configuration energy lowers, because the reactions occur between attracting partials. The final configuration is stable. It consists of the bands of anti-phase boundaries in the initial basal plane and in the planes of cross slip – the prism planes. The model of shear microcracks nucleation in basal planes, with screw ***a***-superdislocations coalescence, takes into account the long-distance elastic interaction of ***a***-superdislocations. The molecular dynamic method was used to study the processes of coalescence of screw ***a***- superdislocations in basal slip band. It is demonstrated, that long-range stress of dislocations in a slip band plays an important part in the process of microcrack nucleation. The formation of short bands of prism slip accompanying the (0001) basal slip was explained. Consecutive coalesce of microcracks in the basal plane results in macrocrack nucleation. Based on the suggested model, the mechanisms of macrocracks formation are discussed.

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