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Simulation of Deformation Behavior at a Crack Tip in Bcc Structural Metals and Alloys

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Summary

Molecular dynamics simulations have been used to investigate the mechanisms of low temperature deformations at the crack tip in bcc structural metals and alloys. Five crack systems with different crack planes and crack fronts are analyzed under opening mode loading conditions. Twinning, new grain nucleation and phase transformation are main deformation behaviors at the crack tip at a high loading rate condition. We notice that there are two different mechanisms of phase transformation for different types of cracks in bcc iron and B2 NiAl. For cracks with $< 100 >$ crack fronts, the bcc (B2)-to-fcc ($L1_0$) martensitic transformation occurs along the Bain path due to the shear stress at the crack tip. Whereas for cracks with $< 110 >$ crack fronts, either the bcc (B2)-to-fcc ($L1_0$) or the bcc (B2)-to-hcp transformation is the candidate. We find that the combination of the local stress and crystal orientation plays an important role on the mechanism of the martensitic transformation. Thus a simple way to determine the mechanism of the martensitic transformation is developed. The complicated deformation behaviors at the crack tip in bcc iron and B2 NiAl are discussed by using this method.

Moreover, based on the studies of the deformation behavior at the crack tip in bcc structural metals and alloys, we find that the crack propagation and the fracture toughness of a material are closely related with the structure evolution at the crack tip region. Crack cleavage usually accompanies with the formation of twinned or martensite strips at the crack tip, while crack blunting occurs due to the dislocation emission or a new grain nucleation at the crack tip. Subsequently, the finite element method is also applied to study the crack propagation behavior in a large scale by introducing the deformation mechanisms in atomistic scale.

References

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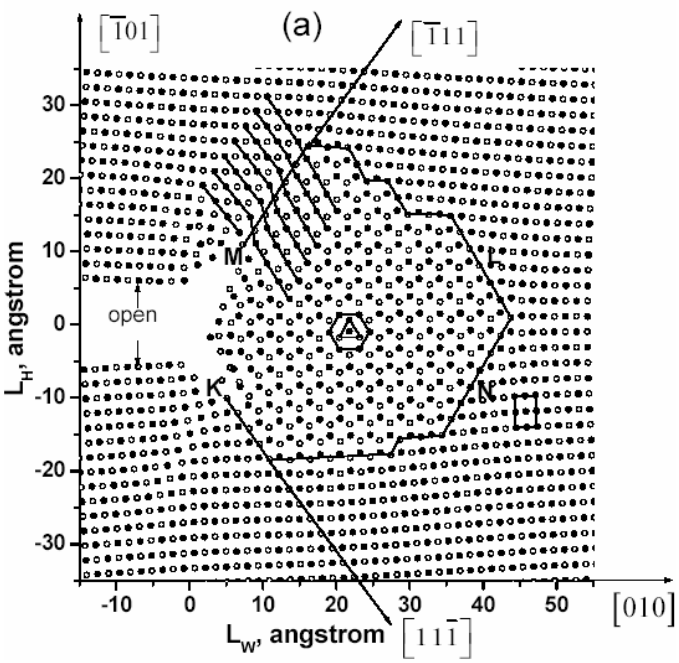

Figure 1: New grain nucleation and phase transformation at the crack tip