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Twin emission and phase transformations in Zr crack tips.

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Abstract – We present atomistic studies of the deformation mechanisms occurring in the crack tip region during low temperature fracture of hcp Zr. Static simulations of mode I fractures on different planes of Zr crystals were performed using empiric embedded atom (EAM) potentials. Depending on the crystal plane and the orientation of the crack on that plane, crack tips advance to different extents and present different tip blunting. Deformation twins appear on every case studied. When the simulation took place with the crack lying in a (0001) basal plane we found a martensitic hcp to bcc phase transformation near the crack tip.

Twinning is an important deformation mechanism in hcp metals at low temperatures and/or high strain-rates. In order to study its influence on Zr toughness, static simulations of fractures on mode I on Zr crystals were performed. We used a molecular static technique (zero temperature) [1] with potentials based on the embedded atom method (EAM) [2]. At each simulation an initially sharp atomic crack is inserted with the crack tip at the middle of the 40000 atoms simulation block; periodic boundaries are imposed in the direction parallel the crack front and displacement boundary conditions at the other two directions are fixed at the desired mode I stress intensity factor K_I according to the elasticity theory. The interior atoms are then allowed to relax to a minimum energy configuration. The applied intensity is increased slowly to simulate an equilibrium quasi-static crack growth.

Cracks were introduced on three different planes of the hcp structure: basal (0001), prism $(1\bar{1}00)$ and pyramidal $(\bar{1}2\bar{1}0)$. For each case two different crack orientations were chosen. Crack tips advanced much more on cracks lying in the $(1\bar{1}00)$ prism plane compared to the other cases. Blunting of the crack tip was more pronounced on cracks lying in the $(\bar{1}2\bar{1}0)$ pyramidal plane. Deformation twins appeared in all cases studied and we compare our results to other simulations [3] where the system was loaded with mixed *K*-fields. On basal cracks we found zones where an hcp to bcc phase transformation took place and we analized the mechanism of such a transformation.

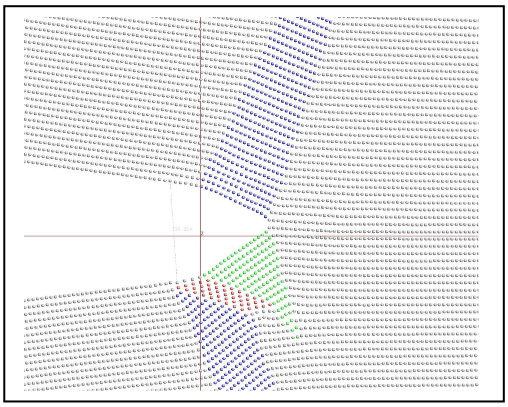

Figure 1: Deformation twins nucleated at the crack tip for a crack lying in plane $(1\bar{1}00)$

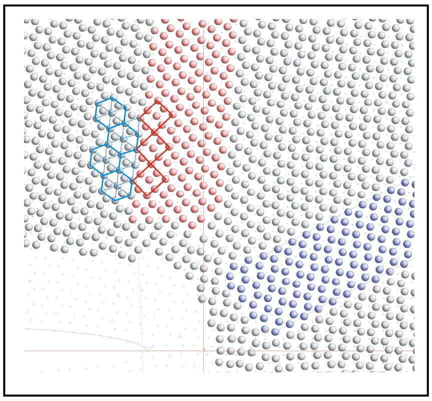

Figure 2: Hcp to bcc phase transformation on a basal plane (0001).

References

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