Temperature induced disorder in ?-Zr

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The behavior of free surfaces and of grain boundaries of a bcc Zr system, close to the melting temperature, are investigated using molecular dynamics in combination with a tight-binding potential. Our system consists in more than 5000 atoms and the potential incorporates both two- and many-body terms. The evolution of the disordering sequence, as the temperature increases, is studied quantitatively and illustrated graphically. We find that a progressive disordering process takes place, both at the free surfaces and at the grain boundary, as the melting point is approached. For these two cases the process turns out to be quite similar.