THERMAL ACTIVATION OF EDGE DISLOCATION UNPINNING FROM OBSTACLES IN IRON

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The mechanical properties of metals are mainly determined by the presence and movement of dislocations. Dislocations can be formed e.g. in fusion or fission reactor wall materials as a result of energetic collision cascades. Hence, studying the movement and interactions of dislocations with other defects in reactor materials is important. Dislocations can be trapped by existing defects, such as point defects, voids, or precipitates. The dislocation pinning strength of different obstacles has been widely studied in atomistic simulations previously. However, few studies have systematically investigated the stress and temperature dependence of the activation energy associated with the dislocation unpinning.

Using molecular dynamics simulations, we study the thermally activated unpinning of an edge dislocation from a void in iron. By applying a constant stress at high temperatures, we systematically measure the activation time of unpinning as a function of the applied stress and temperature. Assuming the thermal activation follows an Arrhenius-like behaviour, we obtain a relation between the activation energy barrier, the applied stress, and the temperature.

We find that the activation energy is dependent on the temperature at constant applied stress. The temperature dependence is found to be largely due to the temperature dependence of the specific shear modulus. A softening of the material at higher temperatures leads to an increase in mechanical work applied on the system, resulting in a lower measured activation energy. The obtained relationship between applied stress, temperature, and activation energy can be useful as input for larger scale simulation methods, such as dislocation dynamics.