Finite temperature influence on the elastic properties of zirconium

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Becuse of its low thermal neutron capture cross section, zirconium based alloys are commonly employed as fuel cladding materials in today's light/heavy water reactor cores. In such environments the material is constantly subjected to the bombardment of high energy neutrons, which collide with primary knock-on atoms and cause microstructural damage in the localized region. This leads to increased concentrations of vacancy and self-interstitial clusters and increased dislocation density. This causes a hardening of the material and an irradiation-induced change in the elastic properties.

The purpose of this work is to model how these properties vary with the amount irradiation damage. To study how these effects influence the material, we resort to classical molecular dynamics (MD) and quantum mechanical density functional theory (DFT). The primary modelling tool of this project is MD, however for benchmarking purposes and to aid the choice of interatomic potential we will use DFT.

The first part of this project and the scope of this presentation is to evaluate the temperature dependent elastic constants for Zr. To achieve this we have conducted DFT calculations within the quasi-harmonic approximation (QHA) at different temperatures, where the Helmholtz free energy is calculated as a function strain from which the elastic constants can be extracted. The elastic properties are then fitted to the universal relation by Varshni[1], which is a semi-empirical relation that is known to describe the elastic properties of solids accurately. In Figure 1 we have compared the DFT calculated results of C_{33} with experimental data[2]. It is seen that the temperature influence on elastic properties are well represented by the DFT model.

We have also used MD to evaluate the temperature dependence of the elastic properties of Zr. For this purpose we tested two different embedded-atom method (EAM) potentials. The MD calculated elastic constant were obtained using a quasi-static approach where the stress tensor is measured as a function of strain. It is found that both potentials approximately capture the temperature dependent elastic constants.

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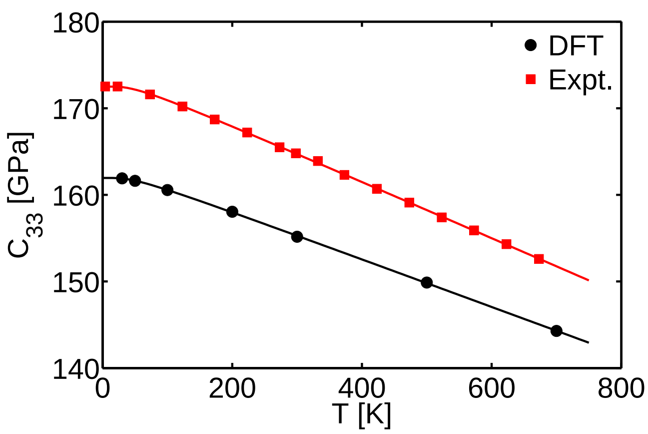

Figure 1: Temperature dependence of C_{33} calculated using DFT compared with experimental measurements. The solid lines represent fits to the Varshni relation.

[1]Y. P. Varshni, *Phys. Rev. B*, **2**, 3952, (1970).
[2]E. S. Fischer and C. J. Renken, *Phys. Rev.*, **135**, A482, (1964).