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Modelling the electronic excitation induced structural dynamics of tungsten

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Tungsten is the leading candidate material for application for the plasma facing wall and divertor in DEMO and future fusion reactors. Here we employ a combination of *ab initio* and empirical simulations to investigate the influence of electronic excitation on the structural response of tungsten to irradiation. We use the high electronic temperature implementation of density functional theory (HTDFT)[1] to investigate phonon dispersion and non-thermal forces in electronically excited tungsten. We observe soft transverse modes in the phonon spectra of bcc tungsten at elevated electronic temperatures (between 10000K and 15000 K) and we find that both fcc and hcp tungsten become dynamically stable at high (> 15000 K) electronic temperatures. Such observations raise the possibility of non-thermal solid to solid phase transitions occurring under conditions of strong electronic excitation.[2]

We have used HTDFT to derive a set of electronic temperature dependent interatomic potentials for tungsten, based on the Finnis Sinclair model.[3] Such potentials include the effects of the change in interatomic interactions associated with the redistribution of the electron density following electronic excitation. They can be employed in two-temperature molecular dynamics (2T-MD) simulations where the electronic energy is coupled to molecular dynamics (MD) and the time evolution of the electronic temperature is calculated by a finite difference solution of the heat diffusion equation.[4] We use the 2T-MD model with the electronic temperature dependent potentials to model the response of a tungsten thin film to laser irradiation. We find that the bcc tungsten film transforms to fcc on the femto-second timescale, prior to transfer of energy from the electronic to ionic systems by electron phonon coupling which subsequently causes the film to melt.

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