

# Multiscale Modelling of Plastic Deformation of Transition Body-Centred-Cubic Metals: From Atomic to Continuum Level

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The topic of this talk is a scheme that links electronic structure and interatomic bonding with atomic level properties of dislocations and via a mesoscopic model of dislocation glide with macroscopic yield criteria applicable on macroscopic level. This development will be demonstrated in the case of plastic deformation of BCC transition metals, specifically molybdenum and tungsten. It is well established that  $1/2\langle 111 \rangle$  screw dislocations in BCC metals possess non-planar cores and, consequently, control the plastic behaviour of these metals. This is the reason why the atomic structure of the cores of these dislocations has been investigated extensively over many years. In this talk we first present results of the recent molecular statics calculations of the structure and glide of  $1/2\langle 111 \rangle$  screw dislocations in Mo and W, performed using the recently developed bond-order potentials. The most important finding of these calculations is a complex dependence of the Peierls stress on the applied stress tensor, in particular its dependence on both shear stresses parallel and perpendicular to the Burgers vector. Based on the results of these atomistic studies we formulate a general yield criterion for the *non-associated flow* that includes the effect of the full stress tensor. This criterion can then be applied when analysing plastic deformation of single crystals in the framework of crystal plasticity and we demonstrate how the yield surfaces in molybdenum and tungsten differ significantly from those based on Tresca or Von Mises criteria that are commonly used in continuum mechanics. However, all these findings are based on calculations corresponding to 0K whilst at finite temperatures the corresponding Peierls barrier is surmounted via the thermally activated formation of pairs of kinks. Theoretical description of this process requires knowledge of the Peierls barrier but this information is not directly obtainable from atomistic studies at 0K. Nevertheless, we show how this barrier, and in particular its dependence on the applied stress tensor, can be extracted phenomenologically from the atomistic studies at 0K. Using the constructed Peierls barrier the strain rate and temperature dependence of the yield stress is then obtained by applying standard dislocation models of the formation of kink pairs. Finally we show that results based on this development are in an excellent agreement with experimental observations of the temperature and orientation dependence of the yield stress in Mo and W.