Electron energy loss spectra near structural defects in TiN and TiC

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In this study, we show how the carbon and nitrogen K-edge fine structures are modified in the vicinity of structural defects in TiN and TiC. Previous results obtained by Scott et al. for stoichiometric TiC [1] have shown that the main peaks of the carbon K-edge spectrum are due to scattering events by the first titanium shell, and by the first and second carbon shells around the absorbing carbon. We try to understand how the structural modifications of these three atomic shells can be responsible for changes in the shape the energy loss spectra in TiN and TiC. To reach this aim, we investigate two kinds of structural defects with the first principles DFT code FEFF8 [2]. In a first part, we calculate the spectrum modifications induced by nitrogen vacancies in TiN, and we show that the shape of the fine structure depends on the position of the vacancies near the absorbing nitrogen. In a second part, we study the spectrum modifications due to stacking faults in TiC. Two different kinds of stacking faults are investigated and we show that changes in the first atomic layers near a stacking fault can be understood in terms of local changes in the electronic structure.

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