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Diffraction, ab-inito calculations and elastic constants of the MAX phases Ti_3XC_2, X=Si,Al

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$M_{n+1}AX_n$ Phase Ceramics are referred to more commonly as MAX phases where M is an early transition metal, A is a group IIIA or IVA element, and X is C and/or N. These materials possess the desirable properties of metals (good thermal and electrical conduction, machinability, and thermal shock resistance) and ceramics (good resistance to chemical attack, oxidation and creep) [1], leading to potential applications in industries such as energy generation, chemical processing, and medicine [2]. The first comparison of an experimentally measured phonon Density of States (DOS) for Ti_3SiC_2 to DFT lattice dynamics and DFT-MD simulation was presented by Kearley et al. [3]. The inelastic neutron scattering (INS) was measured on TOSCA at the ISIS facility using a sample prepared by self-propagating high-temperature synthesis. Above an energy transfer of 25meV the experimentally observed spectrum more closely resembles the MD augmented simulation. From the DFT-MD simulation it can be concluded that the mismatch between spectra is likely due to anharmonic motion or anharmonic atomic potentials between Si and Ti. To further understand the observed mismatch between calculations and experiments the phonon DOS of both Ti_3SiC_2 and Ti_3AlC_2 were taken covering 0-70meV using the PHAROS spectrometers at LANSCE focusing on the low energy regime of the inelastic spectrum, which is closely related to the acoustic phonons. For Ti_3SiC_2, measurements were taken at temperatures of 10, 30, 50 and 70K to allow comparison with DFT lattice dynamics (0K) and DFT-MD (30K, 50K and 70K) simulations. By comparing experimental measurements to simulations and DFT-MD simulations, in particular in case of Ti_3SiC_2, the anharmonic motion of Si in case of Ti_3SiC_2, and apparent harmonic motion of Al in case of Ti_3AlC_2, has been identified.

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