Elastic constants of oriented Ti_3AlC_2 and Ti_3SiC_2 obtained via coherent inelastic neutron scattering

Oliver Kirstein [1,2], Veronica Gray [2,3], Anton P.J. Stampfl [4], and Erich H. Kisi [2]

[1]*European Spallation Source, Sweden*

[2]*University of Newcastle, Australia*

[3]*Swansea University, U.K.*

[4]*Australian Centre for Neutron Scattering, Australia*

Effort has gone into understanding theproperties of MAX phases and their archetypes, Ti_3SiC_2,and Ti_3AlC_2, is as these materials exhibit a desirablecombination of metallic and ceramic properties [1]. Single crystal elastic constants(SEC), usually obtained using *ab-initio*calculations in combination with crystallographic information, indicate thematerials to be isotropic [2]. While it is difficult to obtain single crystalsit is possible to produce highly textured specimens. Using a method developedby Buchenau [3] allows using coherent inelastic neutron scattering to obtain anestimation of the SEC, and such an experiment was performed using thethree-axis spectrometer TAIPAN at ANSTO [4]. Results for Ti_3AlC_2 agree with *ab-initio* calculations and theassumption of isotropy. For Ti_3SiC_2experimental results of c_{44} = 402.7 GPa do not support isotropic valuesobtained from *ab-initio* calculations.Molecular dynamics simulations combined with inelastic neutron scatteringexperiments support the initial diffraction experiment and hence themicromechanical model that was used [5]. We present here a self-consistentdescription of the mechanical properties of the MAX phases $Ti_3SiC_2$and Ti_3AlC_2. [1] M. W. Barsoum et al. Annual Rev.Mat. Res. 41(2011); [2] M. F. Cover et al., J. Phys.Conds. Matt., 21(2009) 305403; [3] U. Buchenau, Sol. St. Comm.,Vol.32(12), 1979 ; [4] V. Gray et al.. J. Am. Ceram. Soc.1-6, 2016; [5] E.H. Kisi et al, J. of Phys.: Cond.Matter 22 (2010) 162202