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The effects of oxygen on Ti2AlC elastic properties: a computational investigation

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The M_2AX phases are a class of nanolaminate materials with a unique combination of ceramic and metallic properties. These materials mimic ceramics in that they are stiff, resistant to oxidation, and remain strong at temperatures exceeding 1400 ^{0}C. The metal like properties of M_2AX phases manifest themselves in their machinability, resistance to thermal shock, high damage tolerance, and electrical and thermal conductivity.[1] This unique combination of properties suggests them as structural materials for demanding operating environments.
M_2AX phases are composed of three elements: an early transition metal (M), a main group element (A), and either carbon or nitrogen (X). They are characterised by a nanolaminate structure in which slabs of the binary carbide/nitride (MX) are separated by single atomic layers of the main group element.
Experimental work on Ti_2AlC, one member of the M_2AX phase family, has shown that oxygen can sit in the carbon lattice position.[2] In addition theoretical work has shown that oxygen atoms can also fill interstitial positions in the aluminium layers.[3] Thus it is important to understand how Ti_2AlC is affected by oxygen incorporation. Using first principles density functional theory we calculate the elastic constants of Ti_2AlC, with oxygen atoms occupying either the carbon sites or aluminium layers, for varying concentrations and configurations of oxygen atoms. By comparing the data from these simulations together with the TiC and TiO elastic constants we are able to explain how oxygen affects the structural and elastic properties of Ti_2AlC.

[1]Barsoum MW, Progress in solid state chemistry, Vol. 28, p. 201-281, 2000
[2]Rosen J et al., Applied physics letters,Vol. 92, No. 064102, 2008
[3]Liao T et al., Journal of materials research,Vol. 24, p. 3190-3196, 2009

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