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Features of a nano-twist phase in the nanolayered Ti_3AlC_2

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Complex intermetallic materials known as MAX phases exhibit exceptional properties from both metals and ceramics, largely thanks to their nanolayered structure. With high-resolution electronic microscopy supported by atomistic modelling, we reveal in this work the formation of a nano-twist phase in the nanolayered Ti_3AlC_2 . We evidence basal pure-twist symmetric boundaries that can be represented by either a screw dislocations networks or pair of disclinations loop.

In this preliminary manuscript, we evidence the formation of a nano-twist phase in the nanolayered Ti_3AlC_2 . High-resolution transmission electron microscopy (HRTEM) with Z-contrast of a Ti_3AlC_2 MAX phase is shown in FIG. 1. The Ti (Al) atomic columns appear as bright white (dark grey) spots and the C atomic columns are not visible. The nano-layered structure of the Ti_3AlC_2 phase is highlighted in the circular inset,

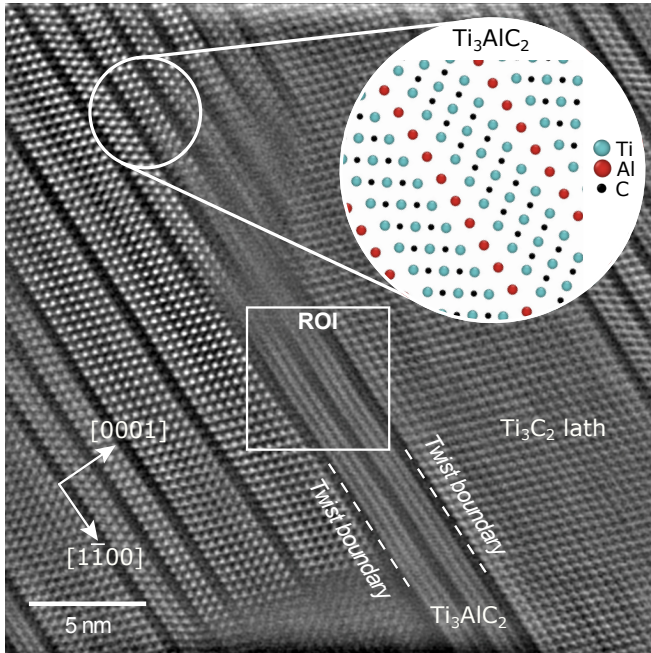


FIG. 1. Experimental observation of the nano-twist phase (region of interest, ROI) in the nanolayered Ti_3AlC_2 . Treated HR-STEM micrography in HAADF mode with electron direction along $[1\ 1\ 20]$. Boundaries of the nano-twist phase are indicated by dashed lines. A model of the Ti_3AlC_2 crystallographic structure is shown in the inset. Some Ti_3C_2 laths are also observed.

with an atomistic configuration. Note the formation of large Ti_3C_2 lath due to the diffusion of Ti within the Al interlayers at high temperature. The region of interest (ROI, white square) shows blurred atomic layers. This indicates a rotation of these particular layers within the basal plane. The boundaries between this rotated phase and the other phase are marked with dashed white lines.

To characterize this rotated region, we reproduce our experimental observation with atomistic simulations.

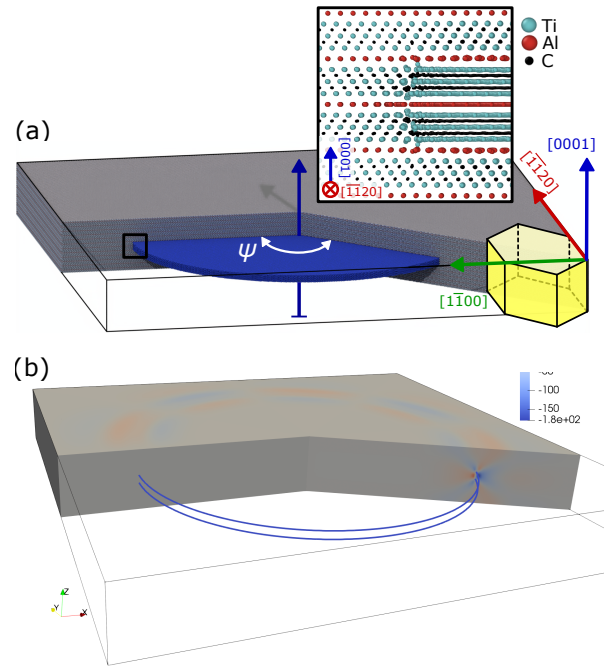


FIG. 2. Modeling of the nano-twist phase in the nano-layered Ti_3AlC_2 by means of a cookie-shape rotation region. (a) atomistic simulation setup of the cookie-shape region (in blue) parallel to the basal planes, with $[000\ 1]$ rotation axis and ψ rotation angle. The black square indicates the location of the inset. : magnified projected view of a 10 nm thick slice of the side of the cookie-shape nano-twist phase for $\Psi = 3^\circ$. Ti, Al and C are colored in green, red and black, respectively. (b) continuum setup of the cookie-shape region defined by a disclination dipole (blue lines).

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FIG. 2(a) shows the atomistic simulation setup to compute the energy and the structure of the rotated phase boundaries. The fully periodic simulation box is made of a bulk Ti_3AlC_2 phase. A region in the center is selected and rotated with an angle Ψ around an axis normal to the basal plane, as indicated in blue in FIG. 2(a). As shown in the inset for a rotation angle $\Psi = 3^\circ$, the configuration obtained with such setup appears similar to the one observed experimentally (FIG. 1).

The modelling of the interface energy and its structures indicate that the interface is similar to a pure-twist grain boundary. This indicate that the defect observed in

FIG. 1 is a nano-twist phase (NTP). For low-angles, the NTP boundary (NTB) can be described by a screw dislocation network. For high-angle, the dislocations forming the network react with each other and cannot be distinguished. We thus observed the formation of complex interfacial reconstructions that appear to be non-monotonously dependant on the twist angle. We find that for high-angles of rotation, the NTB can be accurately represented by a pair of disclinations loop superimposed with out-of-basal-plane eigenstrains (FIG. 2(b)). In particular, the shear stress field shows strong similarity with the one predicted by our atomistic simulations.