157 Understanding Kink Formation of Layered Crystalline Solids with a Focus on Titanium-based MAX Phases

L. Lamberson[1,2a], X. Zhao[1], H. Badr[2], M. Barsoum[2]

[1]Department of Mechanical Engineering and Mechanics, [2]Department of Materials Science and Engineering, Drexel University, 3141 Chestnut Street, Philadelphia, PA, USA

[a] les@drexel.edu

Abstract. Layered crystalline solids, such as graphite, mica, and MAX phases, a transitional metal-ternary carbide or nitride, have basal dislocations that have been assumed as the dominant operational deformation mechanism under load. However, recent efforts on 3D crystalline layered structures have discovered a buckling mechanism that leads to nanoscale rippling deformation, which under further load, forms mesoscale irrecoverable kink banding, giving rise to unique properties at the macroscale. This type of deformation is well documented at larger length scales in other domains such as chevron formation in geology and kinking of laminate composites, to name a few. Consequently, the presented work investigates the unique kinking formation of layered crystalline solids in two ways: via model indention experiments at the macroscale using layers of plastic and metal sheets, and in compression across strain rates of highly orientated MAX phases Ti_3SiC_2 and Ti_2AlC. The idealized macroscale indention studies examine changes in the critical pressure causing buckling, and amplitude and number of modes as a function of layer number, layer thickness, coefficient of friction and level of confinement perpendicular to the layers. These findings are then modeled analytically using linear and nonlinear buckling theory, and provide insight to potentially similar behavior at lower length scales on crystalline layered solids. Additionally, highly orientated MAX phase is used to explore the rate and orientation dependency of kinking of a crystalline solid under quasi-static and dynamic compressive loading using a Kolsky (split-Hopkinson) bar. Noticeable changes in the global stress-strain response of the highly oriented MAX phases are seen as a function of loading orientation, but do not appear to be strain rate sensitive, suggesting that the dominant kinking mechanism is instability driven. Post-mortem scanning electron microscopy (SEM) imaging is used to supplement these findings and aid in discussion.

Introduction

MAX phases are layered, hexagonal carbides or nitrides with the general formula $M_{n+1}AX_n$ where M is an early transition metal, A is a group 13 or 14 on the periodic table, and X is either a carbon or nitrogen [1]. Under ambient conditions, only basal slip is active in these structures, and the layered nature of the microstructure gives rise to ripplocations or buckling at the nanoscale, which leads to nonlinear kind band formation at the mesoscale [2]. This unique instability-driven buckling deformation mechanism gives rise to potentially interesting and useful damage tolerance properties, if fully understood. Consequently, studying model experiments that exhibit similar ripple-to-kink behavior as well as investigating highly oriented MAX phases deformation is imperative to understanding their behavior, and is the focus of this study.

Methods

Model Indentation Experiments

Layers of steel, aluminum or plastic, between 40 to 120 layers deep, were aligned with a 2 mm indenter with its axis parallel to the layers on a universal load frame with a specially created test configuration. By confining the layers perpendicular to the indenter load, the indenter was allowed to penetrate the layers while the confinement force and indenter load was recorded, and reversible buckling (i.e. ripple formation) of certain layers was exhibited. The plastic cards were on the order of 0.3 mm-thick, and the steel and aluminum averaged 0.17 mm-thick, in order to cover a wide range of elastic and plastic constituent properties. In displacement control, the indentation depth was set to fully unload and reload to either progressively higher values to a maximum, or start minimally indented and unload and reload to progressively lower values until a maximum depth (usually around 2 mm) was reached. These nested loops of stress and strain were recorded, energy dissipated per cycle measured, and repeated for various levels of confinement, layer number and thickness, and changing the coefficient of friction to simulate Van der Waals effects (as would be present in crystalline layered materials).

Compression Investigations

In order to investigate compressive loading on layered MAX phases across strain rates, Ti_3SiC_2, the most widely-studied MAX phase to date, and Ti_2AlC was fabricated in highly oriented form. The high degree of orientation means that the majority of the layers (and hence grains) are aligned in the material, in order to more cleanly evaluate the kinking behavior. Prior to this study, no dynamic mechanical investigations of MAX phases have performed on highly oriented microstructures. In this case, compression investigations were carried out both parallel and perpendicular to the layers, in order to bound the problem. Titanium MAX samples on the order of 5 mm cubes were cut by diamond saw and polished to 3 μm on the loading faces. A universal load frame was used to compress samples at 10^{-3} s^{-1} and a Kolsky (split-Hopkinson) bar was used to compress samples at 10^{3} s^{-1}.

Results

The quasi-static compression indentation experiment for the plastic layers with a 400 N confinement is shown in Figure 1 below. In a typical experiment, the initial confining load is applied, and then the indenter is pushed into the layers while recording the displacement. The certain layers proceed to ripple, however it is reversible, as is shown by the nested loops in the figure as the modes of the buckling disappear and reappear per loading cycle. In all cases with all materials examined, as the indenter depth increases, the amplitude of the buckling increases, but the wavelengths remains essentially unchanged. In all cases, the layers recover almost fully upon retraction of the indenter [2].

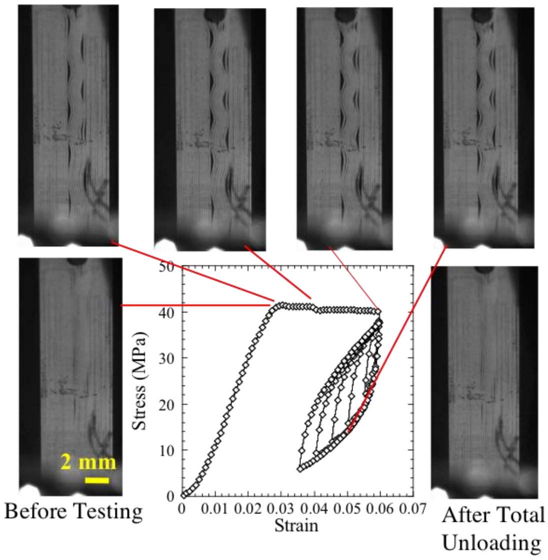

Fig 1. Image of a typical indenter loading cycle on plastic layers, highlighting reversible ripple formation.

For the titanium-based MAX phases, highly oriented Ti_2AlC under dynamic compression (loading in the kinking-induced orientation or in-plane with the layers) reached a peak compressive strength of 1 GPa, whereas quasi-static compression reached a maximum of around 400 MPa. It should be noted that randomly oriented Ti_3SiC_2 exhibits little to no strain rate dependency from quasi-static to dynamic compressive loading, suggesting the improved ability to hold load is due to the texture, likely due to both the interlocking effect of the grains, as well as the favorable orientation for kink band formation. SEM is currently underway to quantify the overall area (and extrapolate to volume) and nature of kink bands in the resulting fragments.

Conclusion

Compression investigations of a titanium-based highly oriented MAX phases show clear changes including an improvement in ability to withstand load, when compared with their randomly oriented microstructures. The complementary buckling investigations using an indenter on layered solids exhibit the same reversible layer ripplocation mechanisms shown in molecular modeling simulations of MAX phase nanolayers [2]. The layered systems scale linearly in terms of energy dissipated per unit volume per cycle of loading as a function of strain, regardless of material system (plastic or metal) investigated, and highlights the important, nonlinear elastic regime that precedes failure of these crystalline layered solids.

References

[1] Barsoum, M.W., *MAX Phases: properties of machinable ternary carbides and nitrides*. John Wiley & Sons, (2013).

[2] Barsoum, M.W., Zhao, X., Shanazarov, S., Romanchuk, A., Koumlis, S., Pagano, S.J., Lamberson, L., Tucker, G.J. 2019. Ripplocations: A universal deformation mechanism in layered solids. *Physical Review Materials,* Vol 3 (2019) p. 1-9.