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Combined FEM and ab initio study on the stabilization of cubic AlN in Ti1-xAlxN/AlN multilayers

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Multilayers that consist of two nanoscale layered materials with the same crystal structure and a small lattice mismatch may grow hetero-epitaxially. AlN has a stable wurtzite structure (w) with hexagonal symmetry and a metastable NaCl structure with cubic (c) symmetry whose mechanical properties are superior from wurtzite phase. In this study, we aim at understanding the fundamental aspects of the phase stability due to the half, fully or partially coherent interfaces combined with the effect of crystallographic and mechanical properties of a substrate. We investigated $Ti_{1-x}Al_xN$/AlN bi-layer system especially by varying the chemical composition of the $Ti_{1-x}Al_xN$ layers systemically from x = 0 to 0.65 where phase transformation (cubic to hexagonal structure) starts, to study the effect of varying coherency strain energy (between the individual cubic $Ti_{1-x}Al_xN$ layers and cubic AlN layers). The elastic energy stored in the system was investigated by finite element method (ABAQUS) in addition to *ab initio* calculations. The results showed that w-AlN phase is preferred for low Al-containing $Ti_{1-x}Al_xN$ layer, but with increasing Al in the $Ti_{1-x}Al_xN$ layer, the growth of cubic-stabilized AlN is preferred initially. These results are helpful to stabilize cubic AlN in a targeted coating design and architecture.

Keywords
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