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Low energy metastable states and immiscibility in $(SiC)_{1-X}$-$(AlN)_X$ BENJAMIN BURTON, NIST, AXEL VAN DE WALLE, California Inst. of Technology, ALBERT DAVYDOV, NIST, VICTOR VINOGRAD, University of Frankfurt, Germany — A cluster expansion Hamiltonian was fit to VASP/PAW calculated supercell formation energies, ΔE_f, and first principles based phase diagrams (miscibility gaps) were calculated for the wurtzite-structure pseudobinary system $SiC_{1-X}AlN_X$. An unusually wide range of $3 \lesssim \Delta E_f \lesssim 125$ kJ/mole MX (M= Al, Si; X= N, C) was calculated and all supercells with $\Delta E_f \lesssim 8$ kJ/mole exhibited characteristic $(SiC)_m(AlN)n$ crystallography, in which $(SiC)_m$ indicates m SiC-double layers $\perp$ to the hexagonal c-axis, and similarly for $(AlN)n$. The prediction of $(SiC)_m(AlN)n$ low-energy metastable states, may explain why one can synthesize $SiC_{1-X}AlN_X$ films, or single crystals of arbitrary bulk composition, in spite of the very strong tendency toward immiscibility. Specifically, one expects that metastable films or single crystals will be dominated by a disordered stacking of SiC- and AlN-double layers.

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