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Melting in two dimensional directionally bonded solids: a Monte Carlo study DONALD PRIOUR, JAMES LOSEY, University of Missouri, Kansas City — We examine melting in two dimensional membranes where there is directional covalent bonding between atomic species, and the bonds are treated as harmonic potentials. We use large scale Monte Carlo simulations to calculate thermodynamic equilibrium variables. We examine square, triangular, and honeycomb lattices for single and dual-layer configurations. The corresponding three dimensional lattices, where long range order is intact, are examined as a reference. We calculate the Root Mean Square (RMS) displacement, finding RMS displacements to vary logarithmically with the system size. Using realistic parameters, we provide quantitative estimates for the RMS displacements for various temperatures. We find swift equilibration times for triangulated systems, but very slow progress toward ergodicity in square and simple cubic systems, a phenomenon similar to the lengthy equilibration times encountered by Fermi, Pasta, and Ulam in the context of anharmonically one dimensional systems.

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