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Computational Modeling of Zinc Blende Crystal Growth JOY HENDRIX, Cornell University — Computational modelling of crystal systems is a useful tool for understanding the mechanisms of crystal formation. Zincblende (cF8-ZnS) was studied as a practice structure because of its relative simplicity, to test the effectiveness of methods that can later be applied to more complex structures, such as spinel. This report discusses principal component analysis (PCA; a machine learning process) and bond angle analysis done on cF8-ZnS trajectories, and also some preliminary studies of spinel (cF56-Al_2MgO_4). The most notable quality of the cF8-ZnS trajectories is that twinned crystal systems form very easily under these parameters. The tests on cF8-ZnS indicate that these ways of analysis are promising for usage on more complex structures, although modifying certain tools, such as the bond angle analysis code, will be useful for further studies on spinel.

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