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A SELF-CONSISTENT ATOMISTIC-PHASE FIELD MODEL FOR THE STUDY OF Ge NANOCRYSTALLIZATION

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In this talk we present a new multiscale model for phase transformation in a heat bath at constant temperature. The model consists on a thermodynamically consistent phase field model that reproduces exactly the interface energetics and kinetics of atomistically computed crystallization fronts. As an additional feature, the interface thickness may be chosen arbitrarily large while preserving this exact atomistic-to-continuum coupling, thus delivering a highly efficient multiscale computational model.

By means of this multiscale approach, we study the interplay between nucleation and growth in the nano-crystallization of amorphous Ge. We find simple scaling laws between the mean radius of crystallized Ge grains, the nucleation rate and the time of crystallization.

REFERENCES

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