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Effects of grain boundary constraints on properties of polycrystalline materials KIMBERLY MCGARRITY, Dept. of Physics & Astronomy, Michigan State University, ERIN MCGARRITY, Dept. of Chemical Engineering & Materials Science, Michigan State University, PHILLIP DUXBURY, Dept. of Physics & Astronomy, Michigan State University, BRYAN REED, Materials and Technology Division, Lawrence Livermore National Laboratories, ELIZABETH HOLM, Computational Materials Modeling, Sandia National Laboratories — Grain boundary networks are engineered by increasing the fraction of boundaries which have favorable properties. Favorable boundaries have either low grain boundary misorientation or they are special boundaries, such as coincident site lattice boundaries. Significant improvement in properties such as corrosion resistance, critical current in superconductors and mechanical strength and toughness occur, provided percolating grain or grain boundary structures can be engineered. We demonstrate that grain boundary constraints shift percolation thresholds from their uncorrelated values and that the behavior near threshold is also modified. The origin of these behaviors is an enhanced clustering of weak boundaries induced by grain boundary constraints.

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