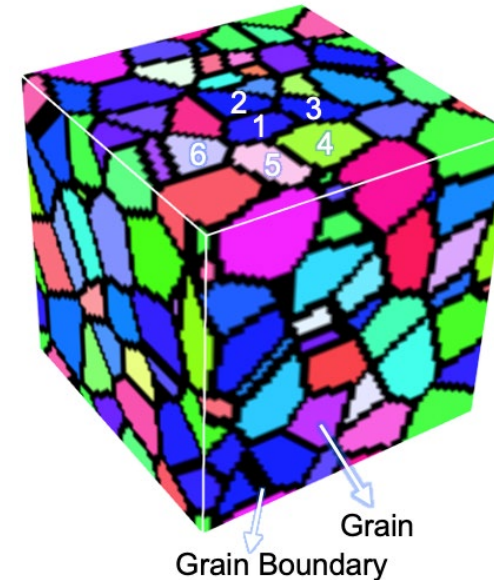


Graph Machine Learning for Polycrystals

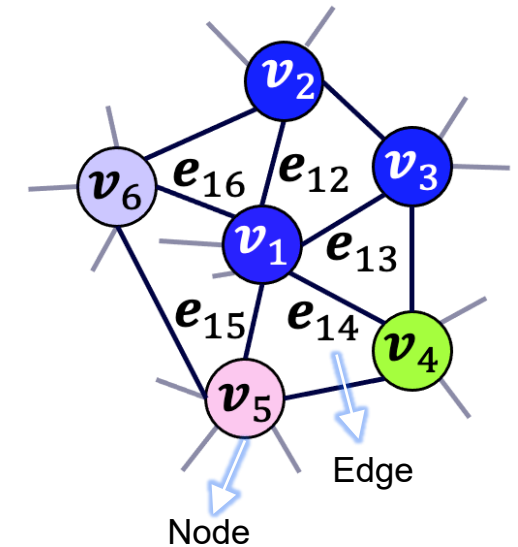
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Polycrystalline materials are everywhere in everyday life, but their microstructure – the arrangement of atoms into crystal grains and grains into a piece of material – covers 10 orders of magnitude in size and involves millions important features. This complexity makes it extremely difficult for scientists to predict the properties of polycrystalline materials quickly and accurately.

Wisconsin MRSEC researchers have leveraged the power of machine learning to tame the complexity of polycrystalline materials and predict their properties. They have developed a graph neural network approach that predicts materials properties with >98% accuracy 90,000 times faster than competing methods. They applied this model to predict magnetostriction, which quantifies the size change of a material induced by a magnetic field. Development and design of high magnetostriction materials will enable MRSEC researchers to efficiently control magnetism using mechanical force and enable future technologies such like magnetic soft robots.



A 3D polycrystalline microstructure model with 133 grains.



A section of the graph encoding this microstructure with 6 nodes and 5 edges. Each node represents a grain and each edge represents a grain boundary.