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Heat Transport in Epoxy Networks: A Molecular Dynamics Study VIKAS VARSHNEY, Universal Technology Corporation, Dayton OH, SOUMYA PATNAIK, BARRY FARMER, AJIT ROY, AFRL, Wright Patterson Air Force Base, OH — In this poster, thermal behavior of a crosslinked epoxy network along with its un-crosslinked counterpart is presented using atomistic molecular dynamics simulations. The simulations were performed on EPON-862 and curing agent-W (DETDA), used as a model system using consistent valence force field (CVFF). The thermal transport is discussed in terms of its thermal conductivity, as calculated using both equilibrium as well as non-equilibrium molecular dynamics approaches, based on Green-Kubo and Fourier law formalisms, respectively. The results are found to be in good agreement with respect to experimental findings. Different energetic contributions of heat flux towards thermal conductivity and their possible coupling in terms of kinetic energy, van der Waals and electrostatic interactions are also discussed. In addition, the broad distribution of low frequency vibrational modes from power spectrum of velocity autocorrelation function suggests their disordered and amorphous nature. The poster also presents heat movement across a crosslinked slab using thermal relaxation simulations and estimates the thermal diffusivity, thermal relaxation time and mean free path for epoxy networks.

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