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Vibrational properties of irradiated nuclear graphite: Inelastic neutron scattering measurements and first-principles calculations

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Research studies into the subject of radiation damage effects in graphite began in the early 1940's as a part of the development of nuclear weapons and nuclear power research. Extensive measurements were performed to study changes to the thermal and mechanical properties of irradiated graphite. Many of these properties such as the thermal expansion coefficient, heat capacity, thermal conductivity, bulk modulus and elastic constants have some level of dependency on the vibrational spectrum. In this work, a series of measurements of the phonon densities of states of different samples of irradiated nuclear graphite were performed at room temperature using the state-of-art Wide Angular-Range Chopper Spectrometer (ARCS) at the neutron spallation source in Oak Ridge National Laboratory. The samples were exposed to different levels of neutron damage (up to $\approx$ 30 dpa) and irradiation temperatures (300–750°C) [1]. The main differences in the phonon dispersion relations and phonon densities of states for samples with different irradiation conditions (damage and/or temperature) are identified. In addition, first-principles phonon density of states calculations of ideal and defected (di- and tetra-vacancy as well as single and di-interstitial) graphite are performed and compared with measured ones.

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Refs

[1] A. A. Campbell, Y. Katoh, M. A. Snead and K. Takizawa, {\it Property changes of G347A graphite due to neutron irradiation}, Carbon {\bf 109}, 860–873 (2016).

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