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# Electronic structure and lattice dynamics of domeykite CU3As according to nuclear quadrupolar resonance of 75As and 63,65CU

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## Abstract

The temperature dependences of nuclear quadrupole resonance (NQR) frequencies, the line width and nuclear relaxation of 75As and 63,65Cu, as well as the electrical resistivity in domeykite Cu3As are studied in the temperature range of 4.2-300 K. The comparison of the calculated with the measured lattice contribution to the NQR frequencies points at a substantial role played by the conduction electrons in creating the electric field gradient at the nuclei sites. The temperature dependence of the copper and arsenic nuclear spin-lattice relaxation linear at $4.2 < T < 200$ K and that of the electric resistivity ($30 < T < 200$ K) prove the metallic character of the conductivity of domeykite. The enhancement of nuclear relaxation, the narrowing of copper and arsenic NQR line widths are considered as arising due to the ionic movement starting beyond 200 K. This movement influences the electric resistivity, most likely due to the inreasing density of states at the Fermi surface.