The Effect of Defects on the Thermal Conductivity of a Graphite Crystal

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Abstract

An analysis is made of the effects of crystallite boundaries and point defects on the thermal conductivity of graphite measured parallel to the basal plane in various approximations. The effects of grain boundaries perpendicular to the basal planes defining a scattering length L_a are estimated using a two dimensional model of a graphite crystal that is neglecting the coupling of the layer planes. This is found to be a good approximation for the "in-plane" vibrations but not for the "out-of-plane" vibrations below $\sim 200^\circ$K. The lattice dynamics of graphite as calculated by Komatsu and Nagamiya(1) are then introduced into a three-dimensional calculation of the conductivity and found to lead to a thermal conductivity at low temperatures varying more rapidly than the specific heat. The temperature dependence, however, is still less than that observed in well crystallised polycrystalline and pyrolytic graphite. The effect of crystallite boundaries parallel to the basal planes defining a scattering length L_c is then investigated and shown to account for at least a part of this discrepancy. An estimate of the c- axis conductivity of a graphite crystal as limited by the boundary scattering also suggests that L_c must be taken into account.

An estimate is made of the effect of point defects on the basal conductivity using the two dimensional model of the graphite crystal. It is found that isotope scattering due to the presence of 1.1% of C^{13} should be observable for L_a values in excess of about 30,000 Å. The magnitude of the scattering of phonons due to vacancies is well able to account for the effects of irradiation on the thermal conductivity of graphite at room temperature and above, leading to the well known stored energy thermal conductivity relation. These estimates are also compared with other experiments on less well crystallised carbons and high temperature measurements of thermal conductivity.

The theory of the crystallite boundary scattering is used to derive values of L_a which can be compared with similar values deduced from the electron and hole mobilities and found to be in reasonable agreement.

Consideration is given to further work on the thermal conductivity of graphite required before a full understanding of this property is reached.

1) Komatsu K, and Nagamiya T. J. Phys. Soc. Japan. 6, p 438 (1951).