Claude A. Klein †

STB Model and Transport Properties of Pyrolytic Graphites*

Structure and texture of pyrolytic graphites (PG) make it unlikely that the three dimensional electron-energy bands of ideal graphite would provide an adequate basis for a discussion of electron transport processes over a broad temperature range.[1] We propose to demonstrate that a coherent description of PG layer-plane phenomena can be based on a parabolic two band system with cylindrical equal-energy surfaces, which are located around the vertical Brillouin zone edges. In this simple two-band model (STB model), band overlap and effective mass must be interpreted as phenomenological parameters to be derived from experiments on highly heat-treated pure PG; with *p*-type (boron doped) specimens, the objective is to describe the situation from the shift of the Fermi level, on the assumption that the presence of trapping centers would not inject major perturbations in the band structure.

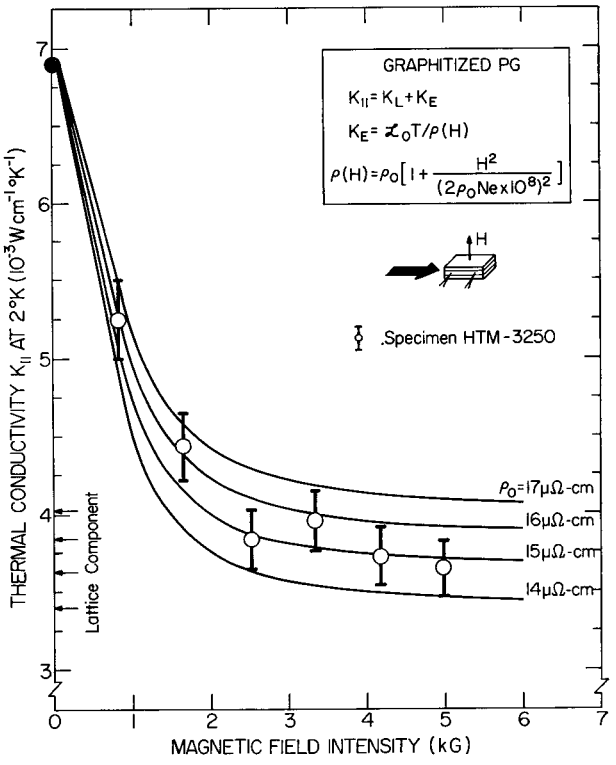
Galvanomagnetic effects

As derived from zero-field resistivity and magnetoresistance mobility, the intrinsic carrier concentration and its variation with temperature in the range 0° to 1500°K implies that past a given graphitization stage band-structural features may no longer be seriously affected by the size of the carbon networks.[2] Above room temperature the carrier concentration increases almost linearly and in accordance with a constant mean effective mass of about 0.025 m_0, which is felt to be compatible with the theoretically predicted distribution of masses along the k_z axis; low-temperature data, on the other hand, suggest an energy-band overlap of 0.01 eV, which may be temperature sensitive through thermal expansion. Band population changes induced by boron doping manifest themselves in the emergence of "metallic" Hall coefficient characteristics, which reflect a shift of the Fermi level away from the Brillouin zone corners.

Thermoelectric effects

In the layer planes of pyrolytic graphite the carrier-mobility behavior is strong evidence for a relaxation time that may be taken of the form $E^{-1/2}$; on this basis it can be shown that the STB model accounts for the Seebeck coefficient, provided that exact Fermi-Dirac statistics are used in conjunction with standard equations for semimetallic systems. In the absence of phonon drag effects, the thermoelectric power yields direct information on the mobility ratio in near-ideal graphite. When electrons are

Figure 1 **Magnetothermal conductivity effect for heat-treated pyrolitic graphite at 2°K.** *The zero-field point is as given by a careful temperature run; measurements made as a function of field strength may have errors of the order of ±5%. The data were taken by M. G. Holland, of Raytheon Company.*



† Raytheon Research Division.

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removed from the upper π band, the Seebeck coefficient follows the predicted pattern and exhibits a sharp positive peak (almost 80 μV/°K at room temperature) in response to the perturbation in the electron-hole balance.

Magnetothermal effects

The recent discovery[3] of a substantial electronic component in the low-temperature thermal conductivity of PG layer planes makes it desirable to develop methods of separating lattice-phonon (K_L) and charge-carrier (K_E) contributions to heat transport in graphite. Saturation magnetothermal conductivity measurements can be successfully utilized for that purpose (see Fig. 1) since, below 4.2°K, we are dealing with a degenerate state of affairs, and the bipolar component is negligible for all acceptable values of the scattering index. How the asymptotic K_L limit is reached as a function of field strength is described within the framework of the proposed band structure model.

References

1. C. A. Klein, *Revs. Modern Phys.* **34**, 56 (1962).
2. C. A. Klein, *J. Appl. Phys.* **33**, 3338 (1962).
3. C. A. Klein and M. G. Holland, *Bull. Am. Phys. Soc.* **8**, 208 (1963).

Discussion

M. S. Dresselhaus: Just because the best pyrolytic graphite appears to have the same carrier mobilities and carrier densities, this does not imply that the band parameters (or at least certain of the band parameters) are the same as for the single-crystal material.

C. A. Klein: I agree. There appears to be evidence from zero-field resistivity data and low-field magnetoresistance data taken on both annealed pyrolytic graphite samples and single-crystal graphite samples that the parameter γ_2, in particular, might be smaller in pyrolytic material than in natural single crystals.