AVERAGING TECHNIQUES IN POLYCRYSTALLINE GRAPHITE

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Previous attempts to theoretically calculate the thermal expansion coefficients and Young's moduli of polycrystalline graphite by averaging over the constituent crystallites have considered only the two limiting approximations of constant stress and constant strain. This study extends the earlier work by using a generalized analysis of crystallite orientation in conjunction with a c-axis accommodation mechanism in an attempt to achieve better agreement with experimental data.

The best agreement with the experimental values of thermal expansion coefficients is given by the constant stress model taking into account c-axis accommodation. Previously, the difference between measurements and values predicted by the constant stress model has been attributed to c-axis accommodation. This accommodation was thought to originate during the cool down from graphitization temperature because of the large anisotropy exhibited by the crystalline thermal expansion coefficients. It was found in this study that the constant stress and constant strain values without accommodation bracket the experimental values. This suggests that a compromise model between the two limiting approximations may partially explain the general trend of the experimentally observed expansion coefficients.

However, the experimental values of Young's modulus do not suggest a compromise between the two limiting approximations. Contrary to the behaviour of less anisotropic materials, the experimental values of Young's modulus are much lower than the average of the values predicted by the two limiting approximations. In fact, they are as low as or lower than the constant stress value. Introducing accommodation does little to bring an average of the two approximations closer to the experimental value but does give better agreement with the value predicted by the constant stress model.

Two modified models are introduced in an attempt to obtain reasonable answers from more consistent models. The first model, referred to as a modified constant strain model, has previously been used to explain the properties of some polycrystalline anisotropic ceramic materials. It consists of a number of columns, formed of two crystallites in series, averaging together as in the constant strain model. The alternative modified constant stress model consists of a constant stress average of crystallite pairs which are formed by connecting two crystallites in parallel as in the constant strain approximation. It has been formulated to supply a mechanism for the introduction of c-axis accommodation into the constant stress model. The modified models represent first attempts toward amalgamating the constant stress and constant strain models.

A numerical evaluation of these modified models gives very good agreement with the experimental results. Values of Young's moduli for these two modified models fall between the two limits of constant stress and constant strain as required by energy considerations. However, they lie very close to the value predicted by the constant stress model rather than the average value of the two limits. Similarly, for the thermal expansion coefficients the predicted coefficients fall between values calculated from the two limiting models. For higher degrees of preferential c-axis orientation the coefficient of thermal expansion predicted by the constant strain model undergoes a rapid increase with increasing c-axis orientation and crosses the value predicted by the constant stress model. This behaviour is reflected in both of the modified models. The overall trend of the predicted values is consistent with experimental observations. Taking accommodation into account gives values in very good agreement with experiment. This agreement suggests that the models represent useful approximations to the structure of polycrystalline graphite.