Raman Study of the Relationship between Microstructure and Physical Properties of Isotropic Graphite

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Abstract. The degree of graphitization, crystallite size, fracture surface and pore morphology of three kinds of isotropic graphite from different companies were characterized by Raman spectroscopy and scanning electron microscopy (SEM). The relationship between physical properties and microstructure was studied.The results showed that the raman values of (I_D/I_G) of three samples were about from 0.32 to 0.47. The flexural strength and electrical resistivity were directly proportional to the value of (I_D/I_G) , while the thermal conductivity was inversely proportional to that value.

Intorduction

Isotropic graphite is a kind of high performance engineering material and indispensable to modern industries. In order to expand its applications, many countries, such as America, Germany, France, Japan et al. have paid great manpower and material resources to develop related technology [1-3].

The microstructure of carbon materials can be characterized by many methods, such as X-ray diffraction, Raman spectroscopy (Raman) and electronic microscopy (including scanning electron microscopy (SEM) and transmission electron microscopy, high resolution transmission electron microscopy, scanning tunneling microscopy, etc.). Among those methods, Raman spectroscopy is one of the mostly used, which is nondestructive and fast, and has a high resolution. For carbon materials, regardless of the structure being simple or complicated, the Raman spectra show only a few prominent features. It results in a few strong spectrum bands with some other affiliated bands. However, their shape, intensities and positions allow researchers to distinguish the form of carbon valence bond, and also deduce the classification of the material and its information about physical properties [4].

In this paper, three kinds of isotropic graphite were selected and characterized by Raman and SEM. The degree of graphitization, microstructure, mechanical properties, electrical properties and thermal properties were compared. According to the characteristics of microstructure from Raman and SEM, the relationship between microstructure and physical properties was discussed.

Experiment

Materials and their properties. Three samples (A, B and C) from different companies were investigated. Some their physical properties are shown in Table 1.
Characterization. Raman measurements were carried out by Thermo scientific DXR with wavelength of 532nm. The fracture surface and pore morphology were investigated using FEI Quanta 200FEG environmental SEM.

Results and discussion.

Raman characterization. For Raman spectroscopy characterization of carbon materials, There are just two intense bands in the range of 1000~2000cm^{-1}. One is around 1350cm^{-1} called D-peak, the other is around 1580cm^{-1} called G-peak. To some extent, the peak intensity ratio of R (I_D/I_G) can represent the degree of graphitization and the crystallite size. The value of R(I_D/I_G) is directly proportional to crystallite size, and inversely proportional to the degree of graphitization [5-6].

The Raman results are shown in Fig.1 and Table 2.

Table 1 Some physical properties of graphite

Sample	Bulk density [g/cm^3]	Elastic modulus [GPa]	Flexural strength [MPa]	Electrical resistivity [μΩ/m]	Thermal conductivity [W/(m · k)]	Coefficient thermal expansion [10^{-6}/K]
A	1.83	10.8	56.8	12	116	5.6
B	1.85	11.6	49.0	10	128	4.6
C	1.84	12.5	65.0	14	90	3.9

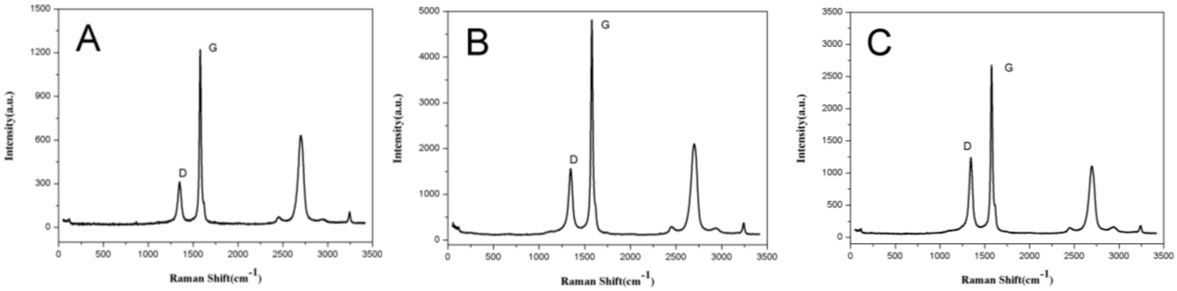

Fig. 1 Raman spectrum of graphite (Samples A, B and C)

Table 2 characterization results of Raman spectrum

Sample	D-peak Position [cm^{-1}]	D-peak I_D	G-peak Position [cm^{-1}]	G-peak I_G	R（I_D/I_G）
A	1337	845.79	1562	2482.08	0.34
B	1345	805.56	1576	2480.63	0.32
C	1345	1405.83	1574	2987.46	0.47

As shown in Fig. 1, in addition to the peak of D (1350cm^{-1}) and G (1580^{-1}), there are two peaks of D* and G* whose frequency is twice of that for the peak of D and G, respectively. The peak amounts and peak position of the three samples are approximately the same, where their intensities are different. As shown in Table 2, the peak intensity ratio order of R (I_D/I_G) for the three isotropic graphite are C>A>B, which also indicates their crystallite size order has the same range and their degree of graphitization order is opposite.

The relationship between R (I_D/I_G) and physical properties. The relationship between R (I_D/I_G) and physical properties could be drawn by setting R (I_D/I_G) as the horizontal axis and flexural strength, electrical resistivity, thermal conductivity as the vertical axis respectively. The curves are shown in Fig. 2.

It can be seen from Fig. 2 that with the increasing of R (I_D/I_G), the flexural strength and electrical resistivity increase, while the thermal conductivity decreases. That is, R (I_D/I_G) is directly proportional to flexural strength and electrical resistivity, while inversely proportional to thermal conductivity.

This can also be seen separately. It is well-known that when the degree of graphitization for graphite is high, the graphite usually has good properties of heat conductivity and electric conductivity. Furthermore, the graphite layers are easy to move with poor mechanical properties. Sample C has the largest amount of R (I_D/I_G), which indicates that it has the lowest degree of graphitization. So it should have the highest mechanical properties of elastic modulus and flexural strength, the lowest heat conductivity and the highest electrical resistivity. These data shown in Table 1 are consistent to the related theory. It is also reasonable to interpret sample B. Sample B has the highest degree of graphitization, and so the best property of heat conductivity and electric conductivity.

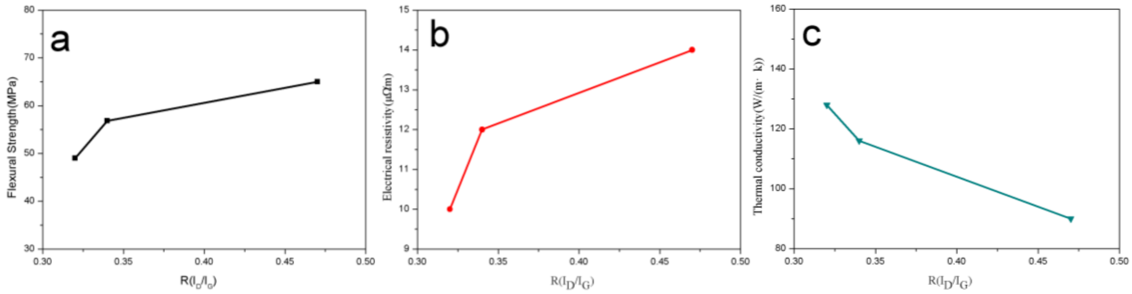

Fig. 2 The relationship between R and flexural strength (a), electrical resistivity (b) and thermal conductivity (c) of samples

SEM characterization. The morphologies of fracture surface of three samples were characterized by SEM under low magnification of 800 and high magnification of 20000, respectively. The results are shown in Fig. 3 and Fig. 4. It can be seen from the images that the particle sizes of sample B and C are well-distributed and smaller than that of sample A, which can interpret that the coefficient thermal expansion of sample B and C is less than that of A.

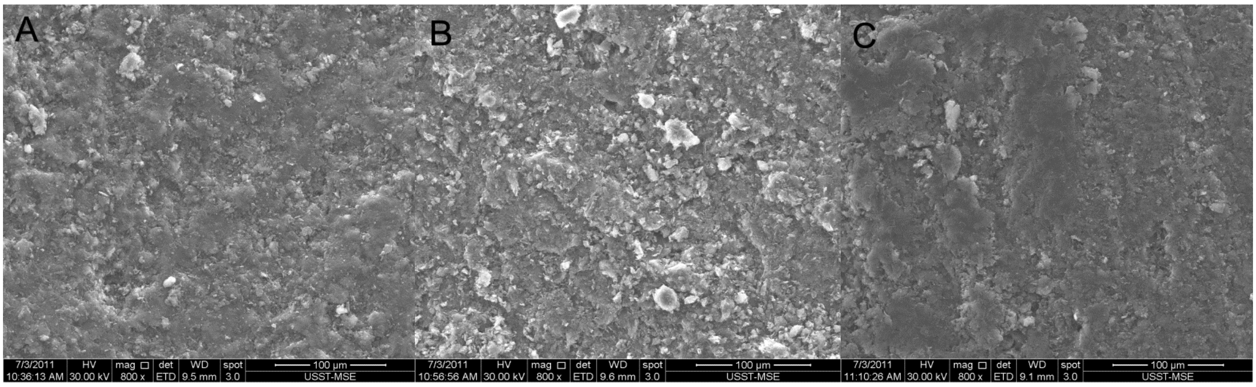

Fig. 3 SEM images of graphite (×800)

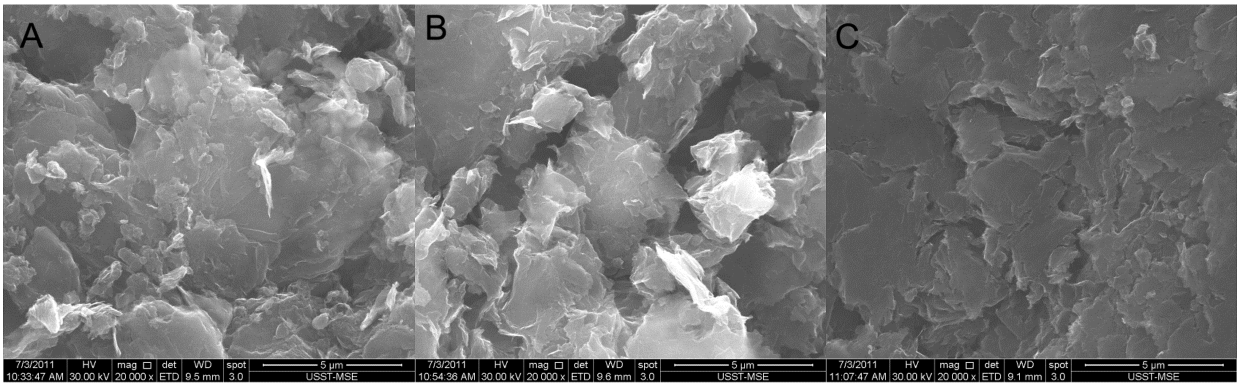

Fig. 4 SEM images of graphite (×20000)

It also can be seen that the pore amounts and size of sample C are smallest. The pore amounts and size of sample B are also larger than sample C, but the partical size is not well-distributed. The surface morphology of sample C is smoothest, with the smallest pore size and pore amounts. So the mechanical property of elastic modulus for sample C is the largest one [7-8].

Conclusions

Microstructure of three different kinds of isotropic graphite was characterized by Raman spectroscopy and SEM. The relationship between microstructure and physical properties was studied. The physical properties of graphite are greatly related to their microstructure, especially the degree of graphitization. The physical properties are also related to size and distribution of the micropores in the graphite. When the degree of graphitization for graphite is high, it usually has good properties of heat conductivity, electric conductivity and poor mechanical properties. When the size of the micropores is small and their distribution is good, the graphite usually has low coefficient thermal expansion and good properties.

Acknowledgements

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