Curie and Pauli Spins in Lithium Intercalated MCMB

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Abstract: The ESR signal of lithium intercalated MCMB can be well simulated by combination of a Lorentz curve and a Gauss curve. The ESR intensity of the Lorentz component is essentially independent of temperature while the Gauss component shows a linear change with the reciprocal of temperature, indicative of Pauli spin and Curie spin, respectively. The former is probably associated with the ordered (graphitized) structures while the latter with the disordered structures in the sample.

Keywords: Lithium intercalation, carbon, ESR, Curie spins, Pauli spins.

The lithium-intercalated carbon was originally a laboratory treasure of physicists, but it has now become the key material for the rechargeable lithium battery, which has the highest specific energy among all known chemical power sources. Although numerous techniques have been invoked to study the structure-property relationship of lithium-intercalated carbons, the problem has not been fully solved so far. There are only a few papers reporting ESR (electron spin resonance) studies of lithium intercalation into carbons[1-3]. We have found that ESR can play a unique role in this aspect. In our previous works, a technique of combined ESR-electrochemical measurements for lithium intercalation into carbon was established[1]. According to the ESR data thus obtained, we were able to deduce the density of electronic states for the carbon and the result turned out to be in reasonable agreement with reported values obtained theoretically or by other experimental methods[4].

Recently,we studied the ESR behaviors of lithium intercalated MCMB (mesocarbon microbeads) and found that the ESR signals are not symmetric in spite of the carbon particles being sufficiently small to prevent the so-called skin effect. The obtained ESR spectra do not fit either Gauss or Lorentz function but can be well simulated by combination of a Lorentz curve and a Gauss curve. The lower part of **Figure 1** shows the two constituent components of the ESR signal and the upper part compares the simulated (the summation of the two components) with the measured spectrum. Variable temperature ESR measurements revealed different temperature dependences for the two constituent ESR signals (**Figure 2**). The ESR intensity of the Lorentz component is essentially independent of temperature while the Gauss component shows a linear change with the reciprocal of temperature, indicative of Pauli spin and Curie Spin respec-tively.

The above data throw a new light on the structure-property relationship of lithiated carbons. The Curie spins and Pauli spins may be attributed to the localized spins and the charge carrier electrons, respectively. Moreover, the former is probably associated with the disordered structures in the carbon while the latter is the ordered (graphitized) structures. This implies that while a great part of the electrons associated with the intercalated lithium ions is added to the Fermi level in the ordered regions, the rest goes to the disordered regions to form isolated spins.

Figure 1 ESR Curve fitting

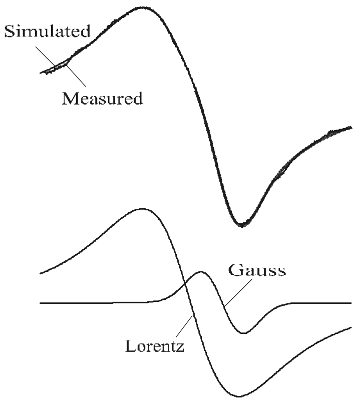
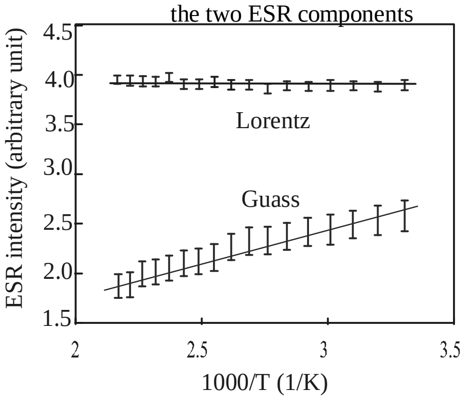


Figure 2 Temperature dependence of the two ESR components



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