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Backscattered electron spectra from graphite

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ABSTRACT

The backscattered electron spectra from graphite sample were studied both experimentally and theoretically at impact energies between 500 and 5000 eV. The angle of the incident electron beam was 50° and the detection angle was 0° with respect to the surface normal, respectively. Monte Carlo (MC) simulations were performed based on the Classical Transport Theory (CTT) model to mimic the experimental spectra. In our simulations, both elastic and inelastic scattering of primary electrons and secondary electron emission from graphite are taken into account. There is found satisfactory agreement between measured and calculated electron spectra.

1. Introduction

The interaction between surfaces and a charged particle plays an essential role in many different areas of research and technology e.g. surface diagnostics and spectroscopy, in understanding of material damage, surface modification (most notably, the possibility of selective desorption and nanostructuring of surfaces by charged particle induced potential sputtering) and in semiconductor devices and plasma-wall interactions.

Electron energy loss spectroscopy (EELS) is used in glancing-angle reflection mode in conjunction with reflection electron microscopy as a technique for studying the composition and atomic coordination in surface layers of crystals [1,2]. EELS has been also used extensively to study the multilayer systems where the thickness of layers is in the nanometer range. These studies have received considerable attention because of its technological interest. On the most fundamental level, its importance is derived from the basic physics that is involved. One key quantities of interest is the response of a many-body system to an external perturbation.

Monte Carlo simulation methods have been playing important roles in materials analysis by electron spectroscopies, electron microscopy, and electron probe microanalysis. A Monte Carlo model with use of bulk (and/or surface) dielectric function has reproduced systematically the backscattering background by taking into account of surface excitation effect in the energy distribution of the direct Auger electron spectra (AES) and the reflection electron energy loss spectra (REELS) [3–6] for a number of elemental materials.

Along this line, the reflection electron energy-loss spectroscopy (REELS) is very important experimental technique for determination of surface phonon dispersion curves of a graphite crystal [1,7]. If we want to understand the interaction of charged particles with matter, we need to be able to measure or predict theoretically what happens with both the particles and the matter with which they interact. A number of experimental studies has appeared [8–11] and a big effort has been devoted to simulate REELS spectra [12–15]. Carbon materials, especially graphite, graphene and carbon nanotubes are of great interest for fundamental and applied studies. The optical properties of graphite have been measured by energy-loss spectroscopy (EELS) techniques [16–18]. Also, in some of our previous study of graphene simple hydrodynamic model were used to explain HREELS experiments [19–23]. In this work the backscattered electron spectra from graphite sample are investigated both experimentally and theoretically at impact energies between 500 and 5000 eV. REELS measurements were performed and our classical transport simulation code was used for the interpretation of the measured data. There was a satisfactory agreement between measured and calculated electron spectra especially for the case of higher incident energies when the surface roughness of the sample and the surface losses are not play significant roles.

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2. Experiment

The graphite (C) sample was used at room temperature in the REELS experiments. The sample cleaning was made by a cold cathode Ar^+ ion gun of AG21 type (Vacuum Generators, UK). The parameters of the ion beam were: the beam energy 2 keV, the incident angle 40° relative to the specimen surface normal and the ion current density 40 μA/cm^2. The cleanliness of the sample surface was monitored by XPS analysis. The atomic percentages of the contaminations were less than 0.5 percent for oxygen (O) and 2 percent for argon (Ar), respectively. In this way the main component of the specimen of C was about 97.7 atomic percent. Such a low level of surface contamination does not give any remarkable features in the energy loss region of the C REELS spectra. A polycrystalline copper (Cu) metal sample was used as a reference specimen for the electron spectrometer energy scale calibration. The energy scale calibration accuracy is about 50 meV, it means the reproducibility. The Cu surface was cleaned by Ar^+ ion sputtering with an ion flux of 120 μA min/cm^2 at 2 keV kinetic energy, at the incidence angle of 40° relative to the surface normal. In the case of the Cu specimen the surface contaminations of C, O and Ar were less than 0.5 atomic percent. The XPS and the high energy resolution REELS measurements were performed in pulse counting mode using the ESA-31 type electron spectrometer developed in ATOMKII [24]. In the REELS measurements, a LEG 62 (VG Microtech, UK) type electron gun was used at five nominal primary electron energies of 0.5 keV (501.5 eV), 1.0 keV (1001.0 eV), 2 keV (1999.5 eV), 4 keV (3997.0 eV) and 5 keV (4995.5 eV). The precise values are not corrected for the recoil effect, which were in our measurement geometry about 0.15 eV at 1 keV and about 0.75 eV at 5 keV for the main component of the specimen of C. The full width at the half maximum (FWHM) of the elastic peak was about 0.6 eV for all the primary energies as it was mentioned above. One part of the FWHM is originating from the electron energy analyzer caused line broadening, which is about 0.5 percent of the analyzer pass energy. The analyzer was working in the fixed retarding ratio mode. The retarding ratios were set up that way the pass energies were about 100 eV at the elastic peak energy. In this way the analyzer caused broadening was about $\leq$0.5 eV. The other main part of the broadening was about $\leq$0.36 eV originating from the primary electron beam. The electron beam caused broadening was coming mainly from the hot tungsten filament heating, so called thermal broadening. In this way a high energy resolution was reached for the elastic peaks. The 0.6 eV FWHM can be calculated from the above mentioned two broadening components by convolution multiplication. The scattering angle of θ_0 was 130° using an angular range of $\delta\theta_0 = \pm 4°$. The angles of the incident and detected electron beams were 50° and 0° degrees measured from the surface normal of the graphite specimen, respectively. The vacuum in the analysis chamber during the REELS measurements was less than 3×10^{-9} mbar.

3. Theory

3.1. Monte Carlo simulation

MC simulation of electron transport in solids is based on the stochastic description of scattering processes. Electron penetration is approximated by a classical zigzag trajectory. Our simulation is based on a well-established electron transport code to model scattering of electrons at surfaces [25]. The elastic and inelastic scattering of primary electrons [25–27] colliding with the graphite surface as well as secondary electron generation inside the material are modeled. Doubly differential elastic scattering cross sections are calculated using the static field approximation with relativistic partial wave analysis [28]. The dielectric response formalism

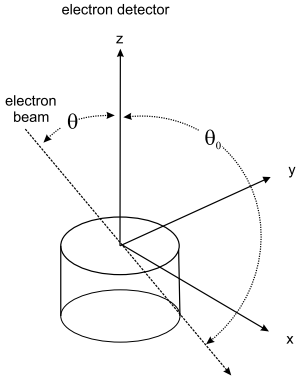

Fig. 1. Schematic view of the experimental and simulation geometric configurations.

[29–31] was used for the description of inelastic scattering cross sections. The energy loss function of graphite is derived from the optical constant [32–34]. In the case of inelastic scattering, a secondary electron is created with kinetic energy equal to the energy loss of the primary electron. Subsequently, the secondary electron trajectory is followed, as well. Initial conditions (starting point, energy, polar and azimuthal angles) for the MC simulation are chosen randomly from suitable distributions to match experimental conditions of the measurements. The scattering point is where the electron changes its direction and/or energy. Particular values of scattering angles of electrons in an individual event are realized by random numbers following the angular differential elastic and inelastic cross sections of the target atom. Fig. 1 shows the geometric configuration used in our experiments and calculations.

3.2. Elastic scattering

After elastic scattering, the scattering angle θ is calculated using the random number $R_1 \in (0, 1)$ satisfying the relation:

$$R_1 = \frac{2\pi}{\sigma_e} \int_0^{\Theta} \frac{d\sigma_e(E,\theta)}{d\Omega} \sin\theta \, d\theta, \tag{1}$$

where σ_e is the total elastic scattering cross-section. A further random number $R_2 \in (0, 1)$ selects the azimuthal angle:

$$\phi = 2\pi R_2, \tag{2}$$

after the elastic collision. The elastic mean free path, λ_e, can be calculated as:

$$\lambda_e = \frac{A}{N_a \rho \sigma_e}, \tag{3}$$

where A is the atomic weight of the target material, ρ is the density and N_a is the Avogadro's number.

3.3. Inelastic scattering

The differential cross section for inelastic scattering in terms of the dielectric function formalism can be written as:

$$\frac{d^2\lambda_{in}^{-1}}{d(\Delta E)\, dq} = \frac{1}{\pi a_0 E} \mathrm{Im}\left[\frac{-1}{\varepsilon(q,\omega)}\right] \frac{1}{q}, \tag{4}$$

where a_0 is the Bohr radius, q is the momentum transfer from an incident electron of kinetic energy E to the solid, causing the energy loss of the incident electron by $\Delta E = \hbar\omega$ and $\varepsilon(q, \omega)$ is the dielectric function as a function of the energy loss and the momentum transfer, respectively. The Penn's expression for calculation of the bulk energy loss function is: