Evaluating the mechanical properties using high beam energy electron energy loss spectroscopy

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Abstract. The electron energy loss spectra of Ge, Si, Cu, MgO, Al, Ni, C (Diamond) were analyzed. The possibility of mechanical parameters of various materials evaluating using bulk plasmon energy in electron energy loss spectra is shown. The bulk modulus of Ge, Si, Cu, MgO, Al, Ni, C (Diamond) is calculated. It is shown that bulk modulus logarithm has a linear correlation with the bulk plasmon energy.

1. Introduction

Determination of mechanical properties of nanostructures is an actual problem of modern materials science [1]. In the first instance, thin films, nanotubes and nanofibers are interesting for investigation [2]. Widely used techniques are acoustic microscopy [3], nanoindentation testing [4], microtensile testing [5], laser ultrasonics [6], micromechanical resonator-based sensing [7].

An original approach to the mechanical properties research of materials without its direct deformation was proposed in [8]. This method is based on bulk modulus calculation using bulk plasmon energy. Bulk modulus allows calculating the Young’s modulus, shear modulus, microhardness, Poisson’s coefficient. This method was developed in [9-11], and applied to a wide class of materials.

In this work the electron energy loss spectra (EELS) of Ge, Si, Cu, MgO, Al, Ni, C (Diamond) were analyzed. The characteristic peaks energies were determined and its origin was interpreted. Bulk modulus of Ge, Si, Cu, MgO, Al, Ni, C (Diamond) were evaluated. The correlation analysis between the bulk modulus and bulk plasmon energy was carried out. It is shown that bulk modulus logarithm has a linear correlation with the bulk plasmon energy.

2. Experimental

According to [8], the bulk modulus $B$ is approximately equal to the product of chemical bond type and squared bulk plasmon energy:

$$B = \alpha \cdot E_p^2,$$

where $\alpha$ depends on the type of chemical bonding, $E_p$ – research material bulk plasmon energy. Two approaches can be used for the bulk modulus calculation:

$$B = 8.44 \cdot \left( \frac{m_e}{h^2} \right)^2 \cdot E_p^2,$$

where $m_e$ is the electron mass and $h$ is Planck’s constant.
\[ B = 7.29 \cdot N_{ve} \cdot \left(\frac{m_e}{h^2}\right)^2 \cdot E_p^2, \]

where \( m \) – effective electron mass, \( e \) – electron charge, \( h \) – Planck constant, \( N_{ve} = n \cdot V_{ws} \) – number of valence electrons, \( n \) – electron density, \( V_{ws} \) – the Wigner-Seitz sell volume. In this paper, formula (2) was used for calculation. The reference values of the bulk modulus \( B_{exp} \) are taken from [9].

EELS from open database [12], including results [13, 14], were analyzed. EELS of Si, Ge, Cu, and C were obtained with transmission electron microscope CM20 PHILIPS. Primary electron energy is 200 keV for Si, Ge, and 100 keV for Cu, C. EELS of Ni, MgO were obtained with transmission electron microscope CM30 PHILIPS at primary electron energy 300 keV.

3. Results and discussion

The initial integral EELS are presented in figure 1. The spectra obtained at high primary electron energies are chosen, since the surface excitations contribution to these spectra is minimal. It simplifies the analysis of bulk origin energy losses.

![Figure 1. EELS.](image1)

![Figure 2. Differential EELS.](image2)

The energy loss spectra main maximum corresponds to the bulk plasma oscillations \( (E_p) \). In the spectrum of C, a low-energy region shoulder is observed. This shoulder is presumably related to a surface plasmon excitation [15]. The spectra (figure 2) were differentiated for more accurately bulk plasmon energy determination. The bulk plasmon energy and structureless background level are shown and marked in figure 2.

The obtained plasmon bulk energies are close to published data [9, 16] and shown in table 1. The table also shows the bulk modulus calculated with the bulk plasmon energy. It is shown that for most of the studied materials, a good agreement between the calculated and reference values of the bulk modulus is observed.

| Element | \( m \) | \( E_p \) (eV) | \( B \) (GPa) | \( B_{exp} \) (GPa) |
|---------|---------|---------------|-------------|-----------------|
| Al      | 1.16    | 15.3          | 75.4        | 75.2            |
| Ge      | 0.66    | 16.5          | 28.4        | 75              |
| Si      | 1.12    | 16.75         | 84.31       | 97              |
| Cu      | 1       | 20.4          | 99.69       | 137.8           |
| MgO     | 1       | 22.0          | 115.94      | 155             |
| Ni      | 1       | 28            | 187.81      | 177.3           |
| C       | 2.12    | 33.75         | 1226.41     | 442             |
All calculated bulk modulus values are presented in figure 3 using logarithmic scale.

![Logarithmic Bulk Modulus vs Bulk Plasmon Energy](image)

**Figure 3.** Bulk plasmon energy dependence of bulk modulus.

The dependence of the bulk modulus on the bulk plasmon energy is well approximated with the linear function \( \log B = 0.07E_p + 0.63 \), and the correlation coefficient is \( R^2 = 0.8 \). Thus, it is possible to determine the elastic properties of materials using electron energy loss spectroscopy. This method can be promising in the development of elastic nanomaterials, the study of the mechanical properties of which is difficult because of its small size.

### 4. Conclusions

The electron energy loss spectra of Ge, Si, Cu, MgO, Al, Ni, C (Diamond) were analyzed. The characteristic peaks energies were determined and its origin was interpreted. The possibility of mechanical parameters of various materials evaluating using bulk plasmon energy in electron energy loss spectra is shown. The bulk modulus of Ge, Si, Cu, MgO, Al, Ni, C (Diamond) is calculated. It is shown that bulk modulus logarithm has a linear correlation with the bulk plasmon energy.

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