

Application of Particular X-ray Standing Wave for Accurate Determination of Electron Density

Oksana V. Pobydaylo, Michael B. Shevchenko, *Institute for Metal Physics, Kiev, Ukraine.*

Study of electron density in crystals is of great interest for understanding a host of their useful properties. We present the new approach for simulation of atomic electron density. The particular standing waves previously predicted for low energy electrons [1], are applied for it. It should be noted, atomic size effects influence position of the nodes of these waves such that the nodes coincide with the atomic planes in the case of 's' scattering. Moreover, formation of such waves leads to minima of intensity of the non-specular reflex. This dynamical effect is similar to multi-beam ones, which happens in the cases of x-ray and high energy electron diffraction [2,3].

In this work, we propose the special scheme for four-beam x-ray Bragg's diffraction, which provides for excitation of the particular standing wavefields. Assuming spherically symmetric model of atomic electron density, it is shown that the sharp changes of intensity of reflected asymmetrically wave, are caused by small varying radius of electron shell. Thus, the particular x-ray standing waves are helpful tool for accurate determination of atomic electron density, whereas the ordinary x-ray standing states are effective for precious determination of interplanar spacing. The particular standing wave effect can be also used to study multilayers and superlattices. In doing so, it is possible to obtain the detailed information about their chemical composition by registering the x-ray diffracted intensity only.

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