m34.p14

Automated Ligand Refinement with a Combined Force Field and Shape Potential

S. Wlodek, A.G. Skillman, A. Nicholls

OpenEye Scientific Software, 3600 Cerrillos Road, Santa Fe, NM 87507, USA.

Keywords: ligand, force fields, shap

An automated computational procedure for fitting a ligand into its electron density with the use of the MMFF94 force field and a Gaussian shape description has been developed. It employs a series of adiabatic optimizations of gradually increasing shape potential. Starting from a set of energy-relaxed ligand conformations, the final results are structures realistically strained to fit the crystallographic data.

m35.p01

The control of x-ray diffracted beam by the surface acoustic wave in the grazing geometry

Gurgen Khachaturyan[a], Levon Levonyan[b]

[a]*Institute of Apllied Problems of Physics, NAS RA, Yerevan, Armenia.* [b]*Yerevan State University, Yerevan, Armenia. E-mail: gurgen@iapp.sci.am*

Keywords: X-ray diffraction, grazing incidence diffraction, surface acoustic wave

The diffraction of X-rays under the small grazing angles of incidence on the surface acoustic wave (SAW) in noncomplanar symmetrical Laue geometry is considered [1]. If the direction of the SAW is along the diffraction vector, the misorientation angle of the reflecting planes from the exact symmetric arrangement as well as the glancing angle of incidence wave locally change along the crystal surface. Of course, the glancing angle of the specularly reflected diffracted wave (SDW) also changes from point to point. These angles are related by $\Phi'_{h2} = (\Phi'_0 - \psi')_2 - \alpha;$, where Φ'_h and Φ'_0 are the local glancing angles of SDW and incidence wave respectively,is the local misorientation angle of the reflecting planes from the symmetric arrangement, α' is the parameter characterizing the local deviation of the incident beam direction from the exact Bragg condition [2].
Both the phase and the amplitude modulations of the SDW due to the diffraction of X-rays on the SAW are discussed. The conditions corresponding to maximal values of the reflection coefficient of the SDW from crystal are found [3].

[1] Sauer W., Metzger T.H., Peisl J., Avrahami Y., Zolotoyabko E.. *Physica B, 1998,* 248, 358.
[2] Aleksandrov P.A., Afanasiev A.M., Stepanov S.A.. *Phys. Stat. Sol.(a)*, 1984, 86, 143.
[3] Cerva H.,. Graeff W.,*Phys. Stat. Sol. (a)* 1984,82, 35.