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Quantitative Study of Inelastic Scattering in Electron Diffraction

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Elastic scattering is the major part of multiple scattering in electron diffraction. However, when inelastic scatterings occur, the Kikuchi pattern appears in electron diffraction. Since the discovery of the Kikuchi pattern by Seishi Kikuchi in 1928, there have been many studies about it. It has long been expected that the quantitative study of Kikuchi pattern would be a method for obtaining various information of materials. However, the quantitative study has been impossible so far because of lack of methods and computing resources for the quantitative simulation of Kikuchi patterns. Furthermore, there has been no good energy-filtering technique to take out separately various inelastic scattering intensities of thermal diffuse scattering (TDS), plasmon and one-electron excitations. Thus, it was impossible to obtain experimental data suited for quantitative analysis of Kikuchi patterns. Recently, energy-filtering techniques have been greatly improved and enable us to obtain Kikuchi patterns found by a certain energy loss. In addition, the development of computing power in recent years has made possible the simulation of Kikuchi patterns. The present study aims to calculate and analyse Kikuchi patterns especially due to TDS.

Up to now, there reported an equation in an original paper of Takagi (*J. Phys. Soc. Japan* (1958) **13** 278), by which band and line features of Kikuchi patterns are explained qualitatively. The equation is correct only in the limiting case where thickness of specimen is large enough. In the present study, a general method for calculating Kikuchi patterns over high angular areas with high angular resolutions has been developed. The patterns simulated by using Takagi's equation and the present paper's equation, and experimental patterns were compared in detail. It is found that the features of asymmetry and detailed interference fringes appear in the experimental patterns, which can be reproduced not by Takagi's equation but by the present paper's equation. In the present study, the Kikuchi patterns are analysed in terms of Bloch wave transitions. It is shown that the excess and defect features of the Kikuchi patterns are interpreted by the strength of inter-branch and intra-branch Bloch wave transitions.

Quantitative comparisons with experimental and simulated Kikuchi patterns has been done for several crystals of MgO, Al and TiO_2, where the Einstein model has been used for the atomic vibration. Quantitatively good agreements between experiments and calculations were obtained, especially for MgO, with changes of thicknesses and directions of incident beam. For Al, quantitatively good agreements were obtained especially for thick crystals where the oxidized surfaces become ineffective. For TiO_2, the geometry of the patterns were well reproduced, but not the intensity distribution, which indicates that the improvement of the atomic vibration model with considering the correlation between the constituent atoms should be taken into account. It is concluded through these analyses that the quantitative method of simulations of Kikuchi patterns has been established by the present work.

The present method for calculating Kikuchi patterns was applied to an analysis of anharmonic atomic vibration in tetragonal $BaTiO_3$. In the electron microscopic image of tetragonal $BaTiO_3$, it is well known that there appears strong contrast in ferroelectric 180-degree domain (M. Tanaka and G. Honjo, *J. Phys. Soc. Japan* (1964) **19**, 954). The origin has been suggested to be inelastic scattering due to TDS, though it has not been verified by numerical calculations. The present study experimentally revealed that the contrast is attributed to atomic vibration modes near Γ point. The contrast was explained by the simulations by TDS intensities using anharmonic potentials of atom vibrations. It is noted that the contrasts are reproduced not by elastic scatterings but only by inelastic scatterings. This indicates that for the phenomena which are not detectable with elastic scatterings, inelastic scatterings can be new probes.