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Kikuchi patterns with temperature diffuse scattering maximums. Robert Karakhanyan, Karine Karakhanyan
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The purpose of the present work is to reveal around Kikuchi lines the temperature diffuse scattering maximums which, to our knowledge, have not been observed before.

As specimen for investigations were single crystalline silicon films prepared by chemical etching of bulk crystals. The transmission electron diffraction Kikuchi patterns were obtained in an EG-100M electron diffraction camera at an accelerating voltage of 100 kV with the primary electron beam almost parallel to [111] and [112] axes. To increase the intensity of temperature diffuse scattering of electrons [1] the Kikuchi patterns from Si were obtained without the benefit of mobile condenser diaphragm.

In the case of the [111] Kikuchi patterns there are Kikuchi lines only with allowed indices. On the contrary in the [112] diffraction pattern besides allowed Kikuchi lines the forbidden excess 222 and deficient 222 Kikuchi lines, which are formed due to Kikuchi electron double diffraction [2,3], are present. It is founded that only along these forbidden Kikuchi lines in vicinity, accordingly, of 222 kinematically forbidden reflections for the excess 222 line and of zero reflection for the deficient 222 line are observed clearly expressed diffuse distributions of intensity. It is showed that these distributions are maximums of temperature diffuse scattering of electrons around Kikuchi lines.

It is clear, that these maximums around Kikuchi lines are analogs of the known maximums of temperature diffuse scattering around diffraction spots. Note also that the maximums of the temperature diffuse scattering are not formed around allowed Kikuchi lines.

It is obtained the diffraction conditions for formation of temperature diffuse scattering maximums around Kikuchi lines. These maximums are symmetric relatively forbidden Kikuchi lines similarly to symmetry of diffuse maximums relatively diffractions spots.

It is disclosed that diffuse maximums around Kikuchi lines are formed when excess 222 line passes through diffraction spots with the same 222 indices and also for very small deviation of the excess 222 line from 222 reflection independent on direction of deviation.

In the Kikuchi patterns obtained with condenser diaphragm the diffuse maximums around Kikuchi lines are not observed.

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Refinement of structural parameters of PbTiO₃ by Convergent-Beam electron diffraction. Roland Schierholz^a, Kenji Tsuda^b and Hartmut Fuess^a

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PbTiO₃ is used as a component in a variety of ferroelectric and relaxor materials with perovskite structure. Calculations by Cohen [1] suggested, the tetragonal phase is stabilized in PbTiO₃, due to Pb-O covalency. Experimentally the charge density in PbTiO₃ has been studied by x-ray powder diffraction confirming the results by Cohen [2,3].

To obtain data from single crystalline areas we use Convergent-Beam Electron Diffraction (CBED). Energy-filtered 2-dimensional data sets including first-order Laue-zones were collected for 14 different incidences around the five zone axis [00-1], [100], [110], [101], [111]. These data sets are used for a refinement of structural parameters such as atomic positions, anisotropic temperature factors and low order structure factors using the program *mbfitpack* [4]. Due to the conversion from electron to x-ray structure factors [5], low order structure factors can be refined with higher accuracy from electron diffraction. We will show the reconstructed 3-dimensional charge density, and discuss the results in comparison to literature.

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