Berry phase in dynamical diffraction theory for deformed crystals

Kei SAWADA[1], Shuichi MURAKAMI[1], Naoto NAGAOSA[1, 2, 3]
[1]The University of Tokyo, [2]CREST, [3]CERC

We develop a theory for a trajectory of an x-ray beam in the presence of a crystal deformation [1]. A dynamical theory for deformed crystals has been investigated by a Takagi-Taupin theory [2]. Such a conventional theory assume incident waves to be plane waves or spherical waves, and concern the propagation of their wave fronts. On the other hand, one can ask what happens if the incident wave is confined in the transverse direction, namely a beam has a finite width whose trajectory is well defined. Naively one might expect that the trajectory of such a beam is always perpendicular to the wave front, which is expected in a conventional geometrical optics derived from Fermat's principle.

We reveal an anomalous behavior of such electromagnetic beams beyond this naïve expectation. We derive a set of equations motion for an x-ray wave packet in the presence of a crystal deformation. Our equations of motion include the dynamical effect and a geometrical phase called Berry phase associated with the wave dynamics. We find that such a Berry phase in deformed crystals gives rise to a shift of the center position of an wave packet. Remarkably, in the vicinity of the Bragg condition, such a coordinate shift is enhanced by a factor $\omega/\Delta\omega$, where ω is a frequency of an x ray and $\Delta\omega$ is an amount of a gap at the Bragg condition. An amount of the enhancement factor can be $\omega/\Delta\omega \cong 10^6$, which implies for example that an atomic crystal deformation gives a macroscopic shift of a wave packet.

Reference:
[1] K. Sawada, S. Murakami and N. Nagaosa, Phys. Rev. Lett. **96**, 154802 (2006).
[2] S. Takagi, J. Phys. Soc. Jpn. **26**, 1239 (1969); D. Taupin, Acta Crystallogr. **23**, 25 (1967).