Debye-Waller factor due to the phase fluctuation in the incommensurate phase: strange behavior in SiO_2

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The effect of phase fluctuation of the modulated structure is discussed. The invisibility of the satellite diffraction in incommnesurate structures was predicted by Overhauser[1]. It is because the Debye-Waller factor due to the phase fluctuation is much larger than that due to phonons. On the other hand, Axe[2] explained why the satellites have been observed by diffraction experiments in many crystals with incommensurate phase. On these two contradictory interpretations, it has been pointed out that proper coordinates should be taken for the calculation of the phase fluctuation[3]. In this paper, we show that in the very close vicinity of the transition, the GPA(Gaussian phase approximation) assumed by Overhauser is valid rather than the GDA(Gaussian displacement approximation) assumed by Axe. Then in some cases it is possible that Debye-Waller factor, though it is not as large as Overhauser predicted, is large enough to prevent the observation of satellite.

The incommensurate phase in quartz(SiO_2) crystal which exists at high temperature ($\sim$ 850K) would be the case. In quartz, the fundamental satellite at $k \sim b/3$ (b is the reciprocal lattice vector) may be missing and the experimentally observed satellite should be the third harmonics of the fundamental modulation. This explains many strange aspects observed in the α-β transition in quartz as described by the new model recently proposed by Aslanyan et al.[4].

1. A.W.Overhauser,*Phys. Rev. B* **3**, 3173 (1998).
2. J.D.Axe, *Phys. Rev. B* **21**, 4181 (1980).
3. T.A.Aslanyan, T.Shigenari and K.Abe,*J. Phys.: Condens. Matter* **10**, 4577 (1998).
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