ON THEORETICAL IMPROVEMENT OF DIFFERENTIAL CROSS SECTIONS FOR INCOHERENT AND COHERENT INELASTIC NEUTRON SCATTERING BY HYDROGEN-BONDED FERROELECTRICS

S.Stamenković

Institute "Boris Kidrič"-Vinča, Beograd, Yugoslavia

Abstract

More rigorous differential cross sections are derived for incoherent and coherent inelastic neutron scattering by hydrogen-bonded ferroelectrics described in the frame of the pseudospin-phonon formalism.

For a direct NS-analysis of the characteristic "interference effect"[1,2] together with qualitative and quantitative behaviour of scattering intensities as functions of the ferroelectric mode parameters[3-5] the tunnelling of active atoms (H,D) and pseudospin(proton)- phonon(heavy ions) coupling are explicitly taken into account. The differential cross sections for incoherent and coherent NS are derived consistently to both the VSK-model[3,4] and the NSV-model[6,7].

The VSK-model (fig.1):

$$\frac{d\sigma^{\pm}_{inc.}}{d\Omega dE'} = \frac{N}{2}\sigma_{inc}\frac{p'}{p}f_q\frac{H}{\omega}g(\omega)\left[\frac{1}{exp(\beta\omega)-1}+\frac{1}{2}\pm\frac{1}{2}\right];$$

$$g(\omega)=N^{-1}\sum_{k}\delta(\omega-\varepsilon_k^{-}); \quad f_q=\left[|F_q''|^2e^{-2W_q''}+|F_q^{\perp}|^2e^{-2W_q^{\perp}}\right];$$

$$F_q=\left[e^{-(\frac{l}{2b})^2}\cos\phi+i\sin(\vec{q}\vec{l}/2)\cdot\sin\phi\right]e^{-b^2q^2/4}; \quad b^2=\frac{\hbar}{m\omega_0}$$

$$tg\,\phi = 2\Omega/(2J_0\langle S_z\rangle) \text{ (Refs. 3-5)}; \quad H=2\Omega\sin^{-1}\phi;$$

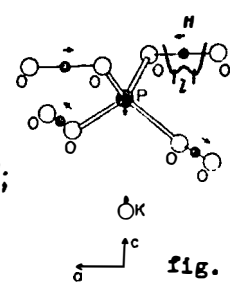

fig. 1

N – the total number of lattice sites.

ω_0 – the classical frequency of one of two coupled linear oscillators within a hydrogen bond.

$$\frac{d\sigma^{\pm}_{coh}}{d\Omega} = \frac{N}{2}\,\sigma_{coh}\, f_{\vec{g}}\,\frac{p'}{p}\left(\frac{1}{exp(\beta\varepsilon^{-}_{q})-1}+\frac{1}{2}\pm\frac{1}{2}\right)\frac{H}{\varepsilon^{-}_{q}}\ ;$$

with a quasi-elastic broadening;[9]

$$\frac{d\sigma_{coh}}{d\Omega} \sim f_{\vec{g}}\,\frac{p'}{p}\,\frac{(k_B T_c)\,H}{P|T-T_c|+Qq^2}\ ,\ \text{at } T\sim T_c\,,\quad \vec{\vec{g}}=\vec{g}-\vec{q}\,,\quad \gamma_q=\pi\Gamma_q^{-}\,.$$

In the above expressions $\vec{q}=\vec{p}-\vec{p}'$ and $\omega=|E-E'|$ is momentum and energy transfers, $\vec{p}$,E and $\vec{p}'$,E' being initial and final wave vectors and energies, respectively; 2Ω is the tunnelling energy of the proton and J_o - an effective proton coupling constant[8] (direct and indirect, through K-PO_4 group); P and Q are parameters of the ferroelectric mode (proton-like)[3-5] ε^{-}_{K}; f_q is an effective pseudospin-Debye-Waller factor[9]; l is the distance between the two minima in a single-particle potential of the proton, m_p - its mass and m - the reduced mass of the K-PO_4 complex, whereas λ^{+}_{o} is the energy gap of the phonon-like mode; the signs +, − stand for the scattering with emission and absorption of the hybridized proton-like mode, respectively, while the indecies ∥ and ⊥ refer to different orientations of hydrogen bonds; besides, the coherent angular cross section above and below are given in the vicinity of a reciprocal lattice vector $\vec{g}$.

The NSV-model:

$$\frac{d^2\sigma^{\pm}_{inc}}{d\Omega\,dE'} = N\sigma_{inc}\frac{p'}{p}\sum_{\alpha=\parallel,\perp}\frac{\sin^2(\vec{q}\vec{l}_\alpha/2)}{m^* l^2}\,e^{-(\vec{q}\vec{l})^2/2}\,\frac{g(\omega)}{\omega}\left(\frac{1}{exp(\beta\omega)-1}+\frac{1}{2}\pm\frac{1}{2}\right);$$

$$\frac{d^2\sigma_{coh}}{d\Omega}\ N\sigma_{coh}\frac{p'}{p}\sum_{\alpha=\parallel,\perp}\frac{\sin^2(\vec{\vec{g}}\vec{l}_\alpha/2)}{m^* l^2}\,e^{-(\vec{\vec{g}}\vec{l})^2/2}\,\frac{(k_B T_c)}{P|T-T_c|+Qq^2}\ ,\ T\sim T_c\,;$$

$$m^* = \frac{V_o(k_B T_c)}{(4\pi)^2 l^2 Q^{3/2}}\,\Gamma(3/2)\zeta(3/2)$$

Here m^* is the effective mass of the proton-like collective excitations ($m^*_H = 3{,}07\ 10^{-26}$ gr; $m^*_D = 10{,}25\ 10^{-26}$ gr); V_o - the volume of the unit cell.

References: 1. H.Stiller, Ber. Bunsenges. Phys. Chem. 72, 94,1968; 2. S.Stamenković, FTT 10,861,1968 /in Russian/; 3. J.Villain, S.Stamenković, phys. stat. sol. 15,585,1966; 4. K.K.Kobayashi, J.Phys. Soc. Japan 24, 497,1967; 5. S.Stamenković, Dynamical Theory of Collective Atomic Motions in Hydrogen-Bonded Ferroelectrics, Thesis, Fac. Nat. Scien. and Math., Belgrade 1975 /in Serbian/; 6. Lj. Novaković, J.Phys. Chem. Solids 31,431,1970; 7. Lj. Novaković, S.Stamenković, A.Vlahov, J.Phys. Chem. Solids 32, 487,1971; 8. P G. de Gennes, Solid State Commun. 1,132, 1963; 9. S.Stamenković, J.Low Temp. Phys. 9,475,485,1972.