Lithium diffusion and C_{60} dynamics by quasielastic and inelastic neutron scattering in $Li_{12}C_{60}$ fulleride

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We have performed inelastic and quasielastic neutron-scattering experiments (IQENS) on the highly lithium doped fulleride $Li_{12}C_{60}$ covering the T range from 150 to 600 K, across a tetragonal to cubic fcc phase transition which was shown to occur around $T = 550$ K by synchrotron x-ray diffraction. In this work we focus on the dynamics of the Li ions and C_{60} molecular units. The QENS data suggest a dynamical model in which the Li ions diffuse in the confined environment of the octahedral void of the pristine C_{60} molecule, in agreement with the structural information that we have obtained on the same compound. These results are discussed together with our previously reported analysis of the changes in the vibrational density of states across the phase transition. The emerging picture is that $Li_{12}C_{60}$ at high temperature (fcc phase) has the same dynamical features as pure C_{60} with the addition of Li localized diffusion within the octahedral void, while the low-temperature tetragonal phase is characterized by a broadening and disappearance of many dynamical features, i.e., of the Li diffusion and of the C_{60} librations and molecular modes.

I. INTRODUCTION

Lithium doping of fullerene has recently attracted special attention[1-3] also because of subtle structural and charge-transfer effects that take place in alkali metal doped fullerenes $A_x C_{60}$ (A = alkali metal, $x = 1,3,4,6, \ldots$) when the radius of the alkali metal is much smaller than the typical radii r of the tetrahedral and octahedral voids of the pristine C_{60} pseudocubic structure ($r = 1.12$ Å and $r = 2.06$ Å respectively). In large radius alkali-metal doped fullerenes (A = K, Rb, Cs) the crystal structure can be modeled (with the only exception of $A_1 C_{60}$) as intercalation of the alkali-metal ions into the pristine C_{60} cubic structure. Moreover these compounds show full electronic transfer from the alkali-metal ion to the C_{60} unit, thus the stoichiometric parameter x reflects the charge state of the C_{60} unit. This class of materials has commanded much interest because of its superconducting and magnetic properties:[4] For instance $A_1 C_{60}$ compounds are cubic at high temperature, while the low-temperature equilibrium phase displays unusual one-dimensional (1D) polymeric chains[5] confirmed by the presence of a distinct inter-C_{60} vibrational signature of polymeric bond.[6,7] Moreover, $A_1 C_{60}$ supports a magnetic spin-density wave transition[8,9] below $T = 50$ K. $A_3 C_{60}$ compounds

display superconductivity [$T_c = 33$ K in Cs_2RbC_{60} (Ref. 10)] with a positive correlation between the critical temperature T_c and the lattice parameter a (which can be varied by choosing the radius of the dopant alkali-metal ion), in agreement with local-density approximation (BCS-LDA) predictions.[11] For all these compounds a natural limit in the doping level is reached at $x = 6$ due to the complete occupancy of the voids of the pristine cubic structure. On the contrary the intercalation with small radius alkali metals (Li and Na, ionic radii = 0.63 and 0.97 Å, respectively) may yield phases with higher alkali-metal content, due to the tendency to form metallic clusters located in the voids of the pseudo-cubic-fullerene structure, as is the case of $Na_{11}C_{60}$.[12,13] In addition, in the case of Na and Li doping there are indications that the charge transfer from the alkali metals to the C_{60} unit is only partial,[13,1] which might imply coordination between the alkali metal and the C_{60} units.

Parrinello and co-workers,[14] based on Car-Parrinello first-principles molecular-dynamics calculations, proposed that $Li_{12}C_{60}$ could be a stable, highly symmetric fullerene cluster, a ''superfulleroid,'' with the 12 Li ions coordinated with the 12 pentagonal faces of C_{60} thus preserving the icosahedral I_h symmetry. Clearly such a system should have an interesting dynamics, in particular due to the coupling of the large C_{60}
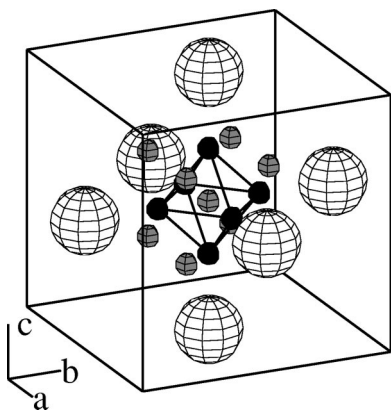
FIG. 1. Li sites in the octahedral void of Li$_{12}$C$_{60}$ at $T = 553$ K from high-resolution x-ray diffraction. The surrounding C$_{60}$ units are indicated as large meshed spheres (whose radius is reduced by $\frac{1}{2}$ for clarity). The C$_{60}$ located at the corners of the unit cell are omitted for clarity. The fully occupied ($4b$ and $32f$) Li sites are indicated by gray balls, and the half occupied sites ($24e$) by black balls, respectively. The outer wire frame is the fcc unit cell, and the inner frame marks the octahedral site.

molecules to the intercalated Li ions: Vibrational, librational, and diffusional motions of both components could mix and influence each other yielding quite complex behavior.

In a previous work[15] we reported the successful synthesis of bulk quantities of different Li$_x$C$_{60}$ compositions, and we have shown that Li$_{12}$C$_{60}$ in the solid state is a single phase compound. With a high-resolution x-ray-diffraction (XRD) experiment[16] we were able to identify its crystalline structure, that is, of an intercalation compound, face-centered cubic $Fm\bar{3}m$ at high temperature ($T = 553$ K) with the Li ions concentrated in the octahedral void of the contracted (lattice parameter $a = 14.089 \pm 1$ Å) fullerene pseudocubic structure. The structure distorts to tetragonal upon cooling below 553 K and stays tetragonal down to 4.2 K. In the high-temperature cubic phase we have obtained strong evidence of coordination between the carbon density on the C$_{60}$ unit and the nearest Li ions. We also found that the Li ions are all grouped in a cluster located at the octahedral void, while the tetrahedral site refines to zero Li occupancy. As shown in Fig. 1, the refined Li sites are: $4b$ (1/2,1/2,1/2) at the centers of the octahedral void; $32f$ $(x,x,x),x = 0.662(1)$, located at the corners of a cube centered in the octahedral voids; and $24e(1/2,1/2,y)$, $y = 0.690(1)$, located at the centers of the faces of the above mentioned cube. While the sites $4b$ and $32f$ refine to full occupancy, the sites $24e$ refine to partial occupancy $N \approx \frac{1}{2}$, which is compatible with diffusion of Li ions between the various $24e$ sites.

The emerging picture for Li$_{12}$C$_{60}$ is that of an hybrid between the superfulleroid cluster, where the Li atoms are attached to the C$_{60}$ unit and therefore show dynamical features similar to those of pristine C$_{60}$ (Ref. 17) (e.g., librations or rotational diffusion) and a *conventional* intercalation compound such as K$_3$C$_{60}$, where the C$_{60}$ units may have some kind of dynamics[18] (typically free rotations or librations) which is, at least in first approximation, decoupled from the alkali-metal vibrational or diffusional processes. In the lower temperature tetragonal phase the lattice parameters contrac-

tion suggests the possibility of the formation of inter-C$_{60}$ polymeric bonds.

In this context we now want to focus on the dynamics of the Li ions in conjunction with that of the C$_{60}$ units, as a function of the temperature. In particular we are interested in the changes of Li diffusion across the tetragonal-cubic phase transition, and how such changes affect the vibrational and librational dynamics of the C$_{60}$ molecules. For this, in principle, IQENS (inelastic and quasielastic neutron scattering) should be an eminently suited technique. There are, however, difficulties, as is common with fullerides, due to the overall weakness of the signal, the combination of the coherent signal from the carbons of C$_{60}$ and the incoherent contribution arising from the ^{7}Li nuclei, and finally the interference of Bragg peaks from the C$_{60}$ crystalline structure, which creates holes in the usable Q space.

In a preliminary work,[19] nevertheless, we have presented data on the changes in the C$_{60}$-originated vibrational density of states across the phase transition. Here we correlate such behavior with changes in quasielastic scattering (QENS), which we were able to model quantitatively; all this leads to a more detailed and specific interpretation of the dynamical changes across the phase transition in this particular fulleride.

II. EXPERIMENTAL

The samples were prepared using the azide decomposition technique.[20] In particular, stoichiometric quantities of purified C$_{60}$ and 99.9% isotopically pure ^{7}Li azide LiN$_3$ were mixed and pelletized in an Ar glove box ($\leqslant 5$ ppm H$_2$O,O$_2$). ^{7}Li purity is required to avoid problems of neutron absorption from the natural fraction of ^{6}Li. More details about the sample preparation can be found in Ref. 15. The samples were then characterized by NMR, XRD, superconducting quantum interference device (SQUID), and Raman spectrometry. Here we just recall that up to 373 K the ^{13}C NMR spectrum shows the full chemical shift anisotropy (about 180 ppm) typical of static fullerides, indicating that the C$_{60}$ rotational dynamics is frozen on the NMR time scale.

Neutron inelastic scattering measurements were performed at the Institut Laue Langevin, Grenoble using the IN6 time-of-flight (tof) spectrometer, operating in neutron-energy gain with incident neutron wavelength of 5.12 Å ($E_i = 3.12$ meV). The 450 mg sample was hosted in a flat, air-tight (sealed with lead wire) aluminum sample holder placed inside the cryoloop. Data were collected at 150, 300, 450, and 600 K. Given the weakness of the signal, in order to obtain an acceptable signal-to-noise ratio we had to use a typical accumulation time of 12 h. The tof spectra were collected over the full range of scattering angles (10.3°–114.2°). Corrections were made for the aluminum can contribution by running an empty sample can. Vanadium was used as a calibrant, allowing determination of the relative efficiencies of the counters. The measured instrumental resolution at the elastic line was on average full width at half maximum (FWHM)=0.10 meV . In order to avoid contamination by elastic (i.e., Bragg peaks) and inelastic (C$_{60}$ lattice phonons) contributions, only six groups, comprising 173 out of a total of 235 tof spectra, were used in the subsequent analysis, as shown in Fig. 2. The average exchanged mo-
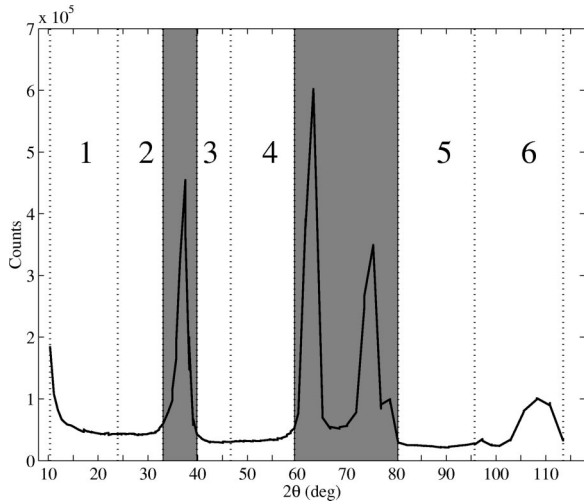
FIG. 2. The diffraction profile of $Li_{12}C_{60}$ measured on IN6 as a function of the scattering angle 2θ at 300 K. The profile is divided into eight different regions, only six of which are not contaminated by elastic contributions and were used in the present study.

menta Q were 0.39, 0.60, 0.89, 1.10, 1.69, and 1.93 Å^{-1} for the six selected regions. From the modeling of the scattering function $S(Q,\omega)$ we could extract the weak quasielastic scattering from the data. The resulting quasielastic scattering function can be then fitted with an appropriate model. In our case we chose a jump diffusion model for the motions of the Li ions in the octahedral symmetry of the voids between the C_{60} molecules.

The neutron-weighted vibrational density of states (DOS) $G(E)$ was obtained summing up the inelastic data from the six regions. Within the framework of the incoherent approximation, the spectral distribution function $P(\bar{\alpha},\beta)$ is given by

$$P(\bar{\alpha},\beta)=2\beta\sinh\left(\frac{\beta}{2}\right)\left(\frac{S(Q,\omega)}{\bar{\alpha}}\right), \qquad (1)$$

where $S(Q,\omega)$ is the uncorrected symmetrized scattering law and the dimensionless variables $\bar{\alpha}$ and β are related to momentum and energy transfer through $\bar{\alpha}=\hbar^2Q^2/2MkT$; $\beta=\hbar\omega/kT$, where M is an average atomic mass. The spectral distribution function $P(\bar{\alpha},\beta)$ was corrected for instrumental background, Debye-Waller, and multiphonon contributions to yield the neutron-weighted vibrational density of states $G(E)$ using the ILL suite of programs. Particular care was used in modeling the theoretical $G(E)$ for the multiphonon corrections at the higher temperatures.

III. RESULTS

A. Vibrational DOS

The C_{60}-originated molecular modes, together with the Li ion excitations are the main features of the vibrational density of states (v-DOS), which is shown in Fig. 3 for $Li_{12}C_{60}$ at $T=600$ K. The vertical bars in the figure mark the positions of the vibrational modes in pure C_{60} as obtained by a variety of techniques: neutron-scattering, Raman, and IR spectroscopy.[21,22] As is usual in this kind of experiment, due to the limited experimental resolution in the neutron-energy-
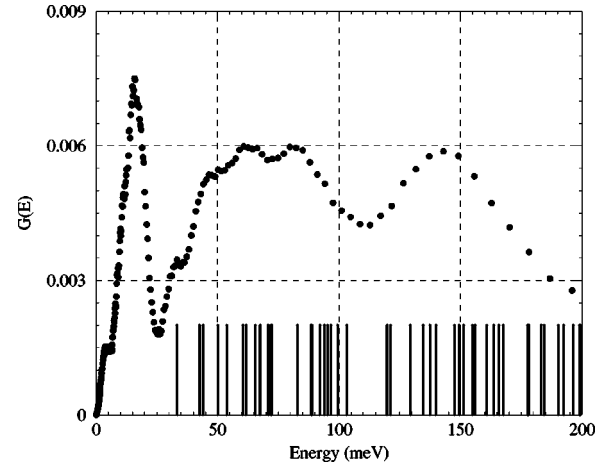

FIG. 3. Neutron-weighted v-DOS measured at $T=600$ K after normalization, background, and elastic peak subtraction and multiphonon correction. The vertical bars mark the modes of pure C_{60}.

gain setup of IN6 and the multiphonon effects (only partly taken into account by the data correction procedure) the C_{60}-originated modes are broadened and overlap resulting in a rather unstructured couple of bunches laying between 30 and 110 meV and between 130 and 200 meV, respectively.

The same v-DOS is detailed in Fig. 4 for the lower energy transfer region as a function of the temperature. Note that the mode originated by the C_{60} "squashing" $H_g(1)$ (33 meV), is distinguishable in the 600 K data set as a shoulder emerging from the broader bunch. The same mode disappears completely in the v-DOS measured in the lower temperature tetragonal phase.

This may indicate that the Li ions clusters act as a "viscous" dampener of the vibrational mode of the C_{60} units, which appear to be freer only at 600 K. In the same figure the broad peak between 10 and 20 meV could be identified with the overlap of Li ion excitations and possibly with vibrations of polymerized C_{60}.

In Fig. 5 we show the scattering law $S(Q,\omega)$ as measured in the first region ($\bar{Q}=0.39$ Å^{-1}) as a function of the tem-
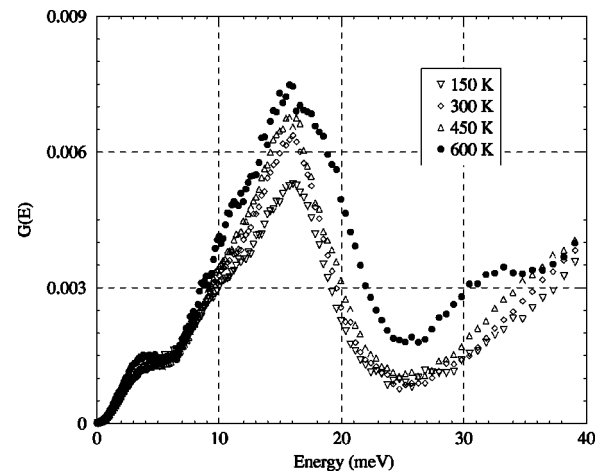

FIG. 4. Low-energy part of the v-DOS as a function of the temperature after normalization, background, and elastic peak subtraction and multiphonon correction.
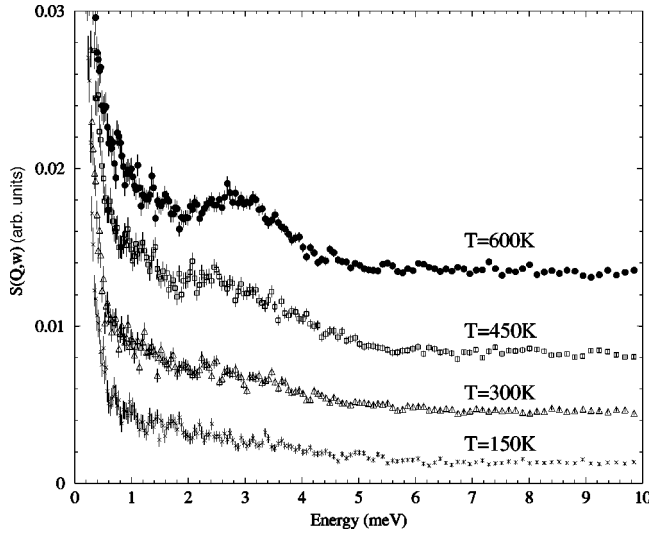
FIG. 5. Scattering law $S(Q,\omega)$ at the lowest exchanged momentum $Q=0.39$ Å^{-1} at the different temperatures marked on the graph. Note the appearance of a well defined excitation at $T=600$ K peaked at 2.8 meV.

FIG. 6. Scattering law $S(Q,\omega)$ measured at $T=600$ K and $\bar{Q}=0.89$ Å^{-1}. The heavier continuous line is the fit model comprising of one Lorentzian QE (light line) and the elastic (dashed line) contributions each convoluted with the instrumental resolution.

perature. In the 600 K data we observe a well defined excitation peak at $E=2.8\pm0.2$ meV with half width at half maximum (HWHM)$=1.0\pm0.2$ meV. Its intensity is much reduced in the $T=450$ K data, while the scattering law is essentially featureless at the lowest temperatures (150 K, 300 K). We identify this feature with the C$_{60}$ librational peak, which is found, e.g., at $E=2.6$ meV in pure C$_{60}$ at 80 K. Its reduction and final disappearance upon cooling implies that the librational motion is dampened at the lowest temperatures in the more compact tetragonal phase, while it is restored in the high T cubic phase. This is a remarkable result since at 600 K, the data show also a restoration of the intramolecular excitation of the C$_{60}H_g(1)$ peak at 33 meV. Survival of the C$_{60}$ librational peak in the high-T phase was already encountered[23] in the case of Na$_2$CsC$_{60}$. Here the case seems to be similar, even if in the lower temperature phase the librational peak vanishes.

B. Quasielastic scattering

The elastic and quasielastic (QE) neutron-scattering intensity was fitted with a two component model, the elastic intensity being represented by a delta function convoluted with the experimental resolution function (given by the vanadium scan) and the QE intensity by a Lorentzian function convoluted with the same resolution function, as is shown in Fig. 6. The intensity of the QE signal decreases on cooling from 600 to 450 K but does not completely disappear even at the lowest temperatures studied. This will be discussed in the following.

The increase of the QE intensity at the tetragonal to fcc phase transition, where the C$_{60}$ units exhibit strongly increased librational motion, indicates that the increased motional freedom of the Li ions is somehow connected with it. However, the librational mode of the C$_{60}$ unit indicates also that the Li ions are not totally free to diffuse between different voids of the C$_{60}$ structure, which would result in a smearing of the reorientational potential felt by the C$_{60}$ units. This
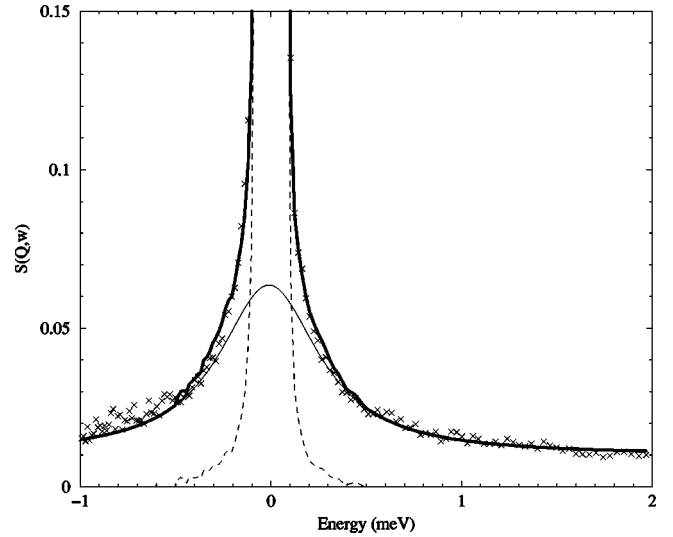
is confirmed by our analysis of the scattering law in the quasielastic range. The first qualitative result we wish to point out is the independence of Q of the width of the QE signal (which is about 0.29 meV, see Fig. 7). At the same time the elastic intensity follows the normal Debye-Waller behavior. In Fig. 8 we report the Q dependence of the ratio of the elastic intensities measured at 600 K versus that at 450 K. This ratio is related to the Debye-Waller factor $I=I_0\exp(-Q^2\bar{u^2})$ associated to Li diffusion. From this we could estimate for the mean-square displacement of the Li ions the value of $\bar{u^2}=0.084\pm0.014$ Å^2, in good agreement with the value of $\bar{u^2}=0.083\pm0.015$ Å^2 obtained from our Rietveld refinement of the high-resolution x-ray-diffraction
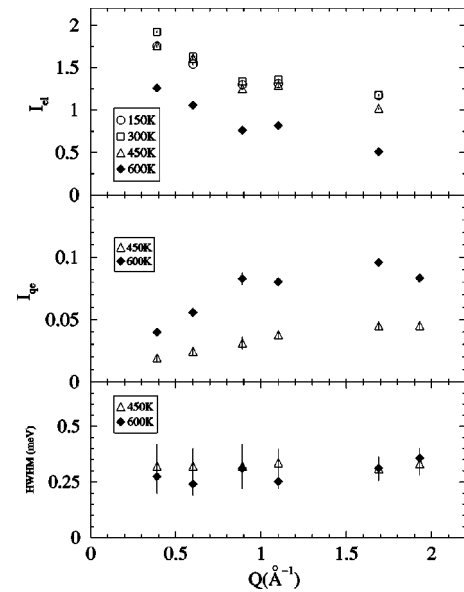

FIG. 7. Elastic (top panel) and quasielastic (middle panel) intensities and quasielastic HWHM as a function of Q for different temperatures in Li$_{12}$C$_{60}$.
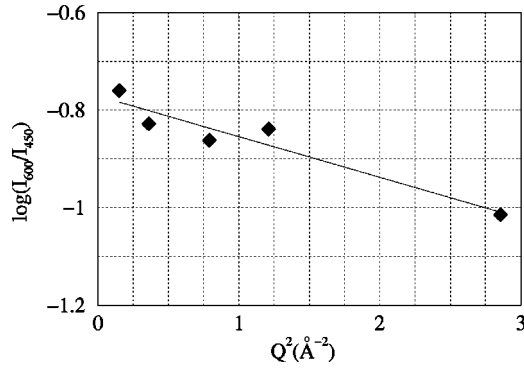
FIG. 8. Q dependence of the ratio of the elastic intensities measured at 600 K versus that at 450 K. Note the logarithmic vertical scale and the quadratic (Q^2) abscissae. The continuous line represents the best fit to the Debye-Waller law, from which we estimate with $\bar{u}^2 = 0.084 \pm 0.014$ Å^2.

data.[16] We used the same Debye-Waller factor to correct the QE intensity, which could then be fitted to a theoretical diffusion model for the the motion of the Li ions. From the Q independence of the QE HWHM we deduce that the diffusional motion must be localized at least when studied on the space scale of the IN6 experiment, that is between 3 and 16 Å from the posed limits on the Q space.

We recall here that in our structural study[16] of the high-temperature $Fm\bar{3}m$ phase of Li$_{12}$C$_{60}$ we found three different sites for the Li ions, all of them within the octahedral void of the pristine fullerenic structure: $4b$ and $32f$ that have full occupancy, and $24e$ [fractional coordinates $(1/2, 1/2, y)$, $y = 0.690(1)$] which has fractional occupancy $N = \frac{1}{2}$. It is therefore reasonable to assume a model in which the Li ions diffuse among the different $24e$ sites (due to their loose occupancy) of a single octahedral void. Within such a model of octahedral jumps in a confined geometry[24] the quasielastic intensity consists of two Lorentzian terms $A_1(Q) = \frac{1}{3}[1 - 2j_0(\sqrt{2}Qr) + j_0(2Qr)]$ and $A_2(Q) = \frac{1}{2}[1 - j_0(\sqrt{2}Qr)]$, where j_0 is the spherical Bessel function of order zero, and r is the radius of the sphere containing the sites. The two QE widths are $\omega_1 = 1.5/\tau$ and $\omega_2 = 1/\tau$, respectively, τ being the residence time of the particle on each site. Even if the two QE terms display different Q dependence, in the Q range of interest to our IN6 experiment, the complete QE scattering function can be approximated—with an accuracy of $\pm 5\%$—to a single Lorentzian of average width $\bar{\omega} = 1.19/\tau$.

In Fig. 9 we show the behavior of the QE intensity, after Debye-Waller correction, for two different temperatures, respectively, below and above the phase transition, and the corresponding theoretical fit, with $r = 2.06$ Å, which coincides nicely with the radius of the octahedral void. From the width of the QE intensity the value of the residence time $\tau = 2.7 \pm 0.5$ ps can be estimated at $T = 600$ K. Here we wish to note that the measured residence time is, within the experimental accuracy, independent of temperature across the phase transition. This indicates that the temperature acts only on the number of ions which diffuse according to the rotational diffusion model we propose; once the Li ions are freed to move, they move with the given mobility determined by the local environment, which changes very little across the
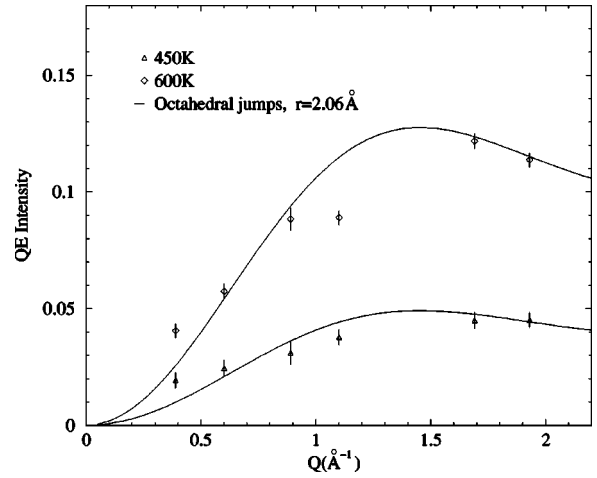

FIG. 9. Q dependence of the QE intensity, after Debye-Waller correction, at $T = 600$ K and $T = 450$ K. The continuous lines represent the theoretical fit to octahedral jumps as described in the text.

phase transition. From the ratio of the quasielastic intensities to the corresponding elastic intensity at 600 and 300 K we find that the number of diffusing Li ions at 600 K is almost five times bigger than at 300 K. In Fig. 10 we overplot the T dependence of the increase of the intensity of the QE signal at $\bar{Q} = 1.10$ Å^{-1} (normalized to the corresponding elastic intensity) with the decrease of the tetragonal distortion of the cubic lattice $[(\sqrt{2}a - c)/c]$ as derived from our XRD study. The two quantities show the same dependence on T. Since the QE intensity is a direct measure of the fraction of Li ions which are free to diffuse, this supports the idea that in the more compact tetragonal phase the Li ions are blocked, while as T is raised the crystal cell expands and more and more Li ions are free to diffuse and therefore contribute to the QE signal. Clearly such mobility should increase at temperatures higher than 600 K, and therefore one should begin to observe some T dependence of the QE width; however, to probe this issue further, higher temperature measurements are necessary.
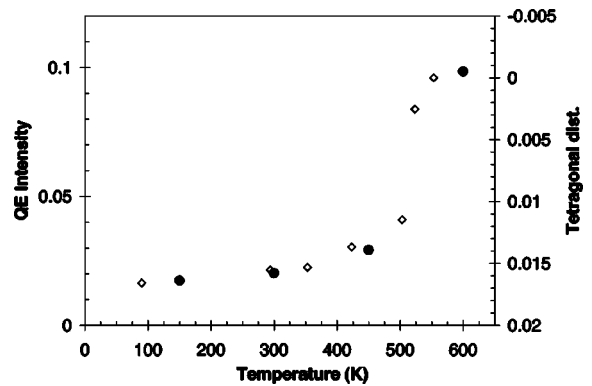

FIG. 10. Temperature dependence of the intensity of the QE signal normalized to the elastic intensity at $\bar{Q} = 1.10$ Å^{-1} (filled circles, left scale) plotted together with the amplitude of the tetragonal distortion of the cubic lattice defined as $(\sqrt{2}a - c)/c$ (empty diamonds, right scale). The latter is plotted in a descending scale. Note that the increase of the QE signal follows the same T dependence as the decrease of the tetragonal distortion.

IV. CONCLUSIONS

The complex dynamics of the highly lithium doped fulleride Li$_{12}$C$_{60}$ has been studied by IQENS. In spite of the difficulties connected with the simultaneous presence of crystalline and disordered system scattering and the weakness of the incoherent scattering signal, we were able to isolate and model quantitatively the diffusional motion of the Li ions across the fcc to tetragonal structural phase transition first detected by synchrotron x-ray diffraction. In particular we propose a localized jump diffusion of the Li ions in the octahedral voids of the Li$_{12}$C$_{60}$ structure. Such motion seems

to be responsible for the previously reported changes in the Li$_{12}$C$_{60}$ vibrational density of states at the phase transition; in particular it explains the observed approach of $G(E)$ to that of pure C$_{60}$, e.g., the restoration of the $H_g(1)$ mode at 33 meV. Higher temperatures studies of QENS may be necessary to probe more quantitatively the diffusional dynamics of the Li ions in Li$_{12}$C$_{60}$.

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