Lattice distortions around frozen and mobile hydrogen in niobium: A molecular-dynamics study

Björn von Sydow and Göran Wahnström

Department of Applied Physics, Chalmers University of Technology and Göteborg University, S-412 96 Göteborg, Sweden

We have studied the hydrogen-induced lattice distortions in niobium using the molecular-dynamics simulation technique. A two-exponential interatomic potential for the H-Nb interaction is proposed, based on recent first-principles calculations for the H/Nb system. The quasielastic diffuse scattering cross section is determined and compared with neutron scattering data. The importance of the hydrogen motion is elucidated by comparing results from dynamic simulations with static defect models and we find that the usual way of introducing the thermal motion of the atoms through a Debye-Waller factor gives a rather imprecise description of the q dependence of the scattering cross section. We also find some evidence that the actual time scale for the hydrogen motion influences the shape of the scattering function at high temperatures (450 K) while at lower temperatures (300 K) this effect is of minor importance. When comparing with the experimental results we find agreement for the q dependence but not for the absolute intensities.

I. INTRODUCTION

Metal-hydrogen systems have been studied extensively during the last decades and basic as well as more applied aspects have been in focus.[1−3] Neutron scattering experiments have provided a lot of information both on the microscopic motion of the hydrogen atom and its isotopes and the accompanying lattice distortion.

One important issue is the proper description of the hydrogen-induced lattice distortion. Only quite recently has it become possible to calculate from first principles the forces exerted by the dissolved hydrogen atom on the surrounding metal atoms and data for interstitial hydrogen in Pd and Nb have been derived.[4] These investigations show that the forces decay reasonable quickly within the range of one lattice constant but are more long ranged compared with some previous estimates.[5]

However, not only are the forces important for the lattice distortion but also the location of the hydrogen atom. Ion-channeling experiments can be used to determine the preferred location,[3] but the assumption that the hydrogen atom statically occupies an individual interstitial lattice site when considering the lattice distortion has been questioned.[6,7] Dosch *et al.*[7] have argued that it is important to take the relative time scale between the hydrogen motion and the lattice relaxation into account. If the hydrogen moves rapidly between different interstitial lattice sites, the lattice distortion may not follow adiabatically the hydrogen motion and this diffusion-induced mechanism has to be taken into account in a proper description of the lattice distortion.

In a previous study[8,9] it was shown that molecular-dynamics (MD) simulations, based on classical mechanics, together with realistic potentials can give detailed microscopic information on the H motion in Nb at high temperatures. It was found that the model could reproduce two key experimental observations: The anomalous Debye-Waller factor and the distinct deviations from simple jump diffusion behavior. Detailed investigations revealed that the H motion is quite complicated and it can move rapidly among several T sites, the sites with tetrahedral symmetry.

In the present study we will concentrate on the diffuse coherent scattering cross section which gives information on the hydrogen-induced lattice distortion. The standard numerical approach to determine the diffuse scattering cross section for randomly distributed defects is based on the formula[10]

$$S_{\text{dif}}(\boldsymbol{q}) = c_D b^2 e^{-2L} e^{-2M} \left\langle \left| \frac{b_D}{b} \exp(i\boldsymbol{q} \cdot \boldsymbol{R}_p) \right. \right.$$
$$\left. \left. + \sum_{m=1}^{N} \left[\exp(i\boldsymbol{q} \cdot \boldsymbol{\delta} \, \boldsymbol{R}_m^p) - 1 \right] \exp(i\boldsymbol{q} \cdot \boldsymbol{R}_m^0) \right|^2 \right\rangle_p ,$$

(1)

where c_D is the concentration of defects, and b_D and b are the coherent scattering lengths of the defects and metal atoms, respectively. The position of the defect is denoted by $\boldsymbol{R}_p$, the undistorted lattice positions by $\boldsymbol{R}_m^0$, and the static displacements of the metal atoms from their undistorted lattice positions (caused by the presence of the defect) by $\delta \boldsymbol{R}_m^p$. The average is taken over all possible defect locations, as indicated by the subscript p. The two factors in front, e^{-2L} and e^{-2M}, are the defect-induced and the usual thermal Debye-Waller factors, respectively. In our case the static Debye-Waller factor can be neglected and the thermal Debye-Waller factor will be determined from the mean-squared displacement of the host lattice atoms. Attempts have also been made[7] to correct for the vibrational motion of the defect by multiplying the factor $\exp(i\boldsymbol{q} \cdot \boldsymbol{R}_p)$ with a Debye-Waller factor. Our results will be presented in dimensionless form by dividing with $c_D b^2$.

The aim with the present study is to determine $S_{\text{dif}}(\boldsymbol{q})$ in Eq. (1) and compare this with an evaluation of $S_{\text{dif}}(\boldsymbol{q})$ from a time-dependent calculation at finite temperatures which resembles the experimental procedure more closely. We can then study to what extent the lattice distortion is influenced by the time scale for the defect motion.

II. INTERACTION POTENTIAL

The necessary input in a MD simulation is a model for the interatomic interactions. In our previous studies[8,9] we have used the Finnis-Sinclair model for the Nb-Nb interaction[11] and a H-Nb potential proposed by Gillan.[12] The former is semiempirical in nature and invokes some many-atom interactions, present in metallic systems. The latter is given as a simple pair potential with two parameters fitted to the two lowest localized vibrational modes for hydrogen. The recent first-principles calculations by Elsässer et al.[4] demonstrate that the H-Nb interaction is more long ranged compared with the model proposed by Gillan. Their calculations also show that the H-Nb interaction depends essentially on the distance between the two nuclei and not so much on the local geometry, i.e., the different interstitial sites for H. It is therefore reasonable to assume a simple pair potential for that part of the interaction.

In the present study we have retained the Finnis-Sinclair model for the Nb-Nb interaction but modified the H-Nb pair potential in order to take the more long-range character of the interaction into account. We have assumed the form

$$V_{\text{Nb-H}}(r) = A\exp[-(r-r_0)/\alpha] + B\exp[-(r-r_0)/\beta], \quad (2)$$

with four independent parameters. These have been determined by fitting to (i) the data by Elsässer et al., (ii) the measured vibrational frequencies, and (iii) the height of the fully relaxed potential barrier when H is displaced from one T site to another. The following values for the parameters were then obtained: $A = 0.4304$ eV, $B = 0.1165$ eV, $\alpha = 0.8791$ Å, $\beta = 0.0759$ Å, and $r_0 = 3.6$ Å.

With this set of parameters we reproduce the forces from the first-principles calculations[4] on the first and second neighboring atoms for a rigid lattice with the H atom located at a T site (1.311 eV/Å and 0.129 eV/Å, respectively). The lattice constant in the first-principles calculations (3.23 Å) is not identical to the lattice constant used here (3.3008 Å) and in the fitting we define the distance to the first and second neighboring atoms in units of the lattice constant. The two lowest localized vibrational frequencies are found to be equal to 119 meV and 189 meV, respectively, which compares well with the experimental numbers [108 meV and 174 meV (Ref. 14)]. These frequencies were determined from the relaxed potential with H located at a T site. This procedure gives very similar results when compared with more appropriate quantum mechanical calculations.[13] The fully relaxed potential energy barrier when H is displaced from one T site to another is equal to 115 meV. This is similar to the barrier in the previous model [122 meV (Ref. 12)] which ensures that a reasonable number for the diffusion constant is obtained.

We also notice that a two-exponential form for the H-Nb interaction has been used previously by Sugimoto and Fukai.[15] They used information on the force-dipole tensor and the vibrational frequency and constructed a potential rather similar to the function in Eq. (2). This early conjecture by Sugimoto and Fukai is therefore now supported by the more recent first-principles calculations by Elsässer et al.[4]
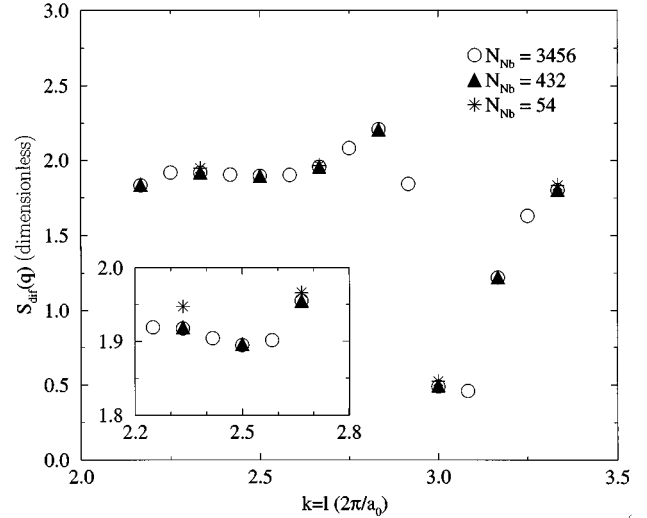

FIG. 1. The diffuse scattering function $S_{\text{dif}}(q)$ calculated along scan 2 ($h = 5/3$) using Eq. (1) with varying system size. $\bigcirc$, 3456 Nb atoms ($m = 12$); $\triangle$, 432 Nb atoms ($m = 6$); $*$, 54 Nb atoms ($m = 3$).

III. SIMULATION DETAILS

In the time-dependent simulation study we are restricted to use a rather small size of the system. To effectively treat an infinite system periodic boundary conditions are employed where the system is replicated throughout space. The allowed q values are therefore restricted by the condition $q = (2\pi/L)(n_x, n_y, n_z)$, where L is the linear size of the system and n_x, n_y, and n_z are arbitrary integers. In the experimental studies by Dosch et al.[7,16] the diffuse scattering cross section is measured along two different scans in reciprocal space. These scans are chosen to obtain maximum information on the local distortion around the defect. We have considered the same quantity and determined the size of the system such that our scattering cross section data are only minutely influenced by the periodic boundary conditions.

We have considered the following two different scans:

$$\text{scan 1: } q_n = \frac{2\pi}{a_0}(h,k,l) = \frac{2\pi}{a_0}\left(\frac{11}{3}, \frac{n}{m}, \frac{n}{m}\right); \quad (3)$$

$$\text{scan 2: } q_n = \frac{2\pi}{a_0}(h,k,l) = \frac{2\pi}{a_0}\left(\frac{5}{3}, \frac{n}{m}, \frac{n}{m}\right), \quad (4)$$

which are close to scan 1 and scan 2 in Ref. 7, respectively. The size of the system is written as $L = ma_0$, where a_0 the lattice spacing ($a_0 = 3.3008$ Å) and n and m are integers. In Fig. 1 we show the result for $S_{\text{dif}}(q)$ along scan 2. These values have been determined with a single static H atom located at a T site and with the surrounding Nb atoms fully relaxed to their distorted equilibrium positions. An average is made over six different configurations with H located at the six inequivalent T sites. To test the size dependence we have considered three different values for m, $m = 3$, 6, and 12, and we find that the results are surprisingly insensitive to the size of the system. Using $N_{\text{Nb}} = 432$ ($m = 6$) or $N_{\text{Nb}} = 3456$ ($m = 12$) metal atoms leads to essentially the same result. This clearly shows that $S_{\text{dif}}(q)$ for these particular q values is dominated by the local distortion around the defect and not

on the long-range distortion field which is always present in an elastic medium and is inevitably influenced by the periodic boundary conditions. We have verified that the same conclusion also holds for the q values along scan 1.

In the subsequent time-dependent calculations we will use $N_{Nb}=432$ metal atoms and one H(D) atom. This small size of the system will make it feasible to perform rather extensive time-dependent calculations.

We have also investigated to what extent the H motion is modified by the change of the H-Nb interaction, compared with the studies in Refs. 8,9. Due to the fact that both the vibrational frequencies and the fully relaxed potential energy barrier for diffusion are roughly the same, we do not expect any large change. The diffusion constant for deuterium is found to be slightly lower, $D_s=3.81\times10^{-5}$ cm^2 s^{-1} at 450 K, compared with $D_s=5.78\times10^{-5}$ cm^2 s^{-1} at the same temperature.[9] This difference is not surprising considering the fact that the *magnitude* of the diffusion constant depends sensitively on the height of the potential barrier for diffusion. We can compare these numbers with the experimental value which is equal to $D_s=1.97\times10^{-5}$ cm^2 s^{-1} at 450 K.[3] The wave vector dependence of the integrated intensity of the quasielastic peak has also been determined and we find a very similar "anomalous Debye-Waller factor" as in Ref. 8. From this we conclude that the details of the H motion, as revealed in the previous study,[8] are quite unaffected by the present change of the H-Nb interaction.

IV. RESULTS

We will now determine $S_{dif}(q)$ from a time-dependent calculation at finite temperatures in a way that resembles the experimental procedure as closely as possible. Experimentally the scattering intensity is measured for a given wave vector transfer q and energy transfer $\hbar\omega$, convoluted with the experimental resolution function. The diffuse scattering cross section $S_{dif}(q)$ is obtained as the (quasi)elastic intensity at constant q. The data are corrected for by subtracting the background intensity and the incoherent scattering caused by the deuterium atom. Absolute intensities are obtained by normalizing to the scattering from a known host lattice phonon.[7]

In our case, the output data from the MD simulation are used to determine the intermediate scattering function,

$$F(q,t)=\left\langle\left[\frac{b_D}{b}e^{i\,q\cdot R_p(t)}+\sum_n e^{i\,q\cdot R_n(t)}\right]\left[\frac{b_D}{b}e^{-i\,q\cdot R_p(0)}+\sum_m e^{-i\,q\cdot R_m(0)}\right]\right\rangle,\qquad(5)$$

where R_p denotes the position of the deuterium atom and R_n, $n=1,\ldots,N$, the positions of the Nb atoms. The coherent scattering lengths are equal to $b=7.1$ fm and $b_D=6.7$ fm for Nb and D, respectively. By dividing with b^2 we have written $F(q,t)$ in a dimensionless form. We have also determined the same scattering function for pure Nb at the same temperature,

$$F^0(q,t)=\left\langle\left[\sum_n e^{i\,q\cdot R_n^0(t)}\right]\left[\sum_m e^{-i\,q\cdot R_m^0(0)}\right]\right\rangle,\qquad(6)$$

and subtracted that quantity from the total function,

$$\Delta F(q,t)\equiv F(q,t)-F^0(q,t).\qquad(7)$$

To obtain the diffuse scattering cross section the Fourier transform of $\Delta F(q,t)$ is integrated together with a Gaussian resolution function $R_G(\omega)$,

$$S_{dif}(q)=c_D b^2\int_{-\infty}^{\infty}\Delta F(q,\omega)R_G(\omega)d\omega,\qquad(8)$$

where

$$R_G(\omega)=\exp[-\ln2(2\omega/\Delta\omega_0)^2].\qquad(9)$$

The full width at half maximum of the resolution function is chosen to have the same value as in the experimental study,[7] $\hbar\Delta\omega_0=3.8$ meV.

First we have determined $S_{dif}(q)$ using Eq. (1). In this case the deuterium atom is held fix at a T site and the surrounding Nb atoms are allowed to relax to their distorted equilibrium positions. No thermal motion is included. The calculation is repeated for the six inequivalent locations of the deuterium atom and the quantity $S_{dif}(q)$ is derived. The thermal motion of the metal atoms is added by including the thermal Debye-Waller factor e^{-2M}, following Eq. (1). In the present case the defect-induced static Debye-Waller factor e^{-2L} is close to unity and can be neglected. The following numbers are used: $b_D=6.7$ fm, $b=7.1$ fm, and $\langle u_{Nb}^2\rangle=5.9\times10^{-3}$ Å^2, where $M=\frac{1}{2}q^2\langle u_{Nb}^2\rangle$. The mean-squared displacement for the metal atoms, $\langle u_{Nb}^2\rangle$, is obtained from a MD simulation for pure Nb at 450 K. The results are shown in Fig. 2, denoted as "static."

We can now compare these data with a full MD calculation where $S_{dif}(q)$ is determined using Eq. (8). In this case the diffusive and vibrational motion of the deuterium atom is included automatically as well as the distortions and vibrations of the Nb atoms. The results depend on the temperature and in Fig. 2 we present our data for 450 K, "$m=m_D$."

The main difference between the cases "$m=m_D$" and "static" is that in the time-dependent calculation the deuterium atom is allowed to move. The assumption behind Eq. (1) is that the rapid local vibrations should show up in a time-averaged fashion and be effectively included in the thermal Debye-Waller factor e^{-2M}. Other motions should be too slow compared with $\Delta\omega_0^{-1}$ and should not influence $S_{dif}(q)$. Attempts have been made to multiply the factor $\exp(i\,q\cdot R_p)$ in Eq. (1) with an "effective" Debye-Waller factor to take into account the fact that the amplitude for the vibrational motion is not the same for Nb and D.[7] However,
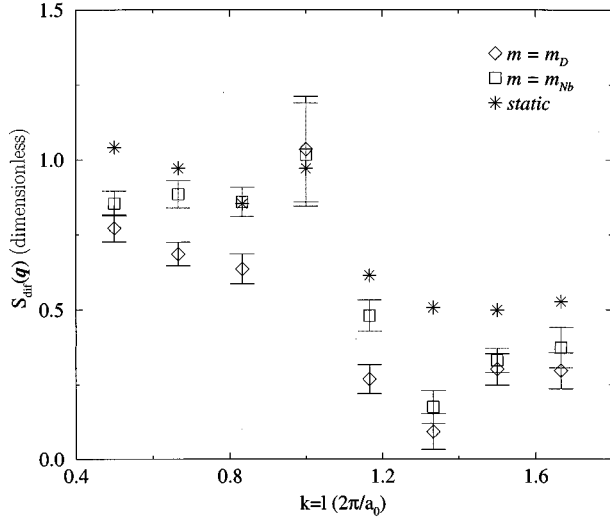
FIG. 2. The diffuse scattering function $S_{\mathrm{dif}}(q)$ at 450 K calculated along scan 1 ($h=11/3$). $\Diamond$, obtained from a MD simulation; $\Box$, obtained from a MD simulation but where the mass of the defect is artificially increased to the mass of the metal atoms; $*$, obtained from a static calculation with the thermal Debye-Waller factor added. The error bars represent an estimate of one standard deviation.

with reasonable numbers for the "effective" Debye-Waller factor rather small effects on $S_{\mathrm{dif}}(q)$ are observed.[7]

Next we would like to investigate if the *time scale* for the defect motion is important for the difference between the cases "$m=m_D$" and "static" shown in Fig. 2. If that is the case a proper calculation of $S_{\mathrm{dif}}(q)$ has to include time-dependent lattice distortions, where the time-dependence is given by the motion of the defect. On the other hand, it can also be that treating the location of the defect fixed at a T site and adding the deviations from this position *only* through a Debye-Waller factor may be too crude. We can to some extent distinguish between these two different aspects of the defect motion by changing the mass of the defect in the time-dependent calculation but keeping the *same* expression for the interatomic potentials. In that way we *only* influence the relation between the time scale for the defect and lattice motion but the averaged instantaneous spatial configurations of all atoms will be the same. (The latter statement is true provided the system is ergodic which we assume to be true.)

We have considered two different masses for the defect, the true mass ("$m=m_D$") and equal to the mass of the metal atoms ("$m=m_{\mathrm{Nb}}$"). The case "$m=m_{\mathrm{Nb}}$" corresponds more closely to the situation with a static defect, with respect to the motion of the lattice atoms, but where the actual spatial correlation between the defect and the surrounding metal atoms is treated in a proper way. By increasing the mass with a factor $m_{\mathrm{Nb}}/m_D=46.5$ the typical vibrational frequency and the mean thermal velocity are reduced by a factor $\sqrt{m_{\mathrm{Nb}}/m_D}=6.8$. We also expect the diffusion constant to be reduced by about a factor $\sqrt{m_{Nb}/m_D}$ and from the simulation we obtain the factor 5.1; the diffusion constant is reduced from $D_s=3.81\times10^{-5}$ cm^2 s^{-1} to $D_s=0.744\times10^{-5}$ cm^2 s^{-1}. In both cases we use identical interatomic potentials. The result is shown in Fig. 2.

We notice that the difference between the cases "$m=m_D$" and "$m=m_{\mathrm{Nb}}$" is not large but for several q val-
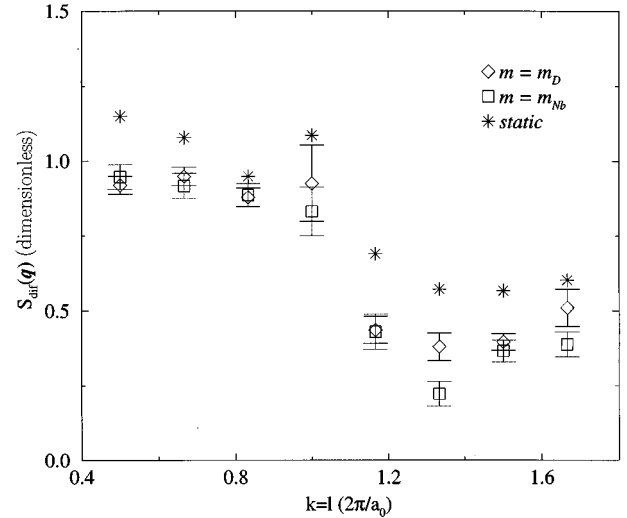

FIG. 3. The same as in Fig. 2 but at 300 K.

ues the two numbers deviate from each other. The error bars represent an estimate of one standard deviation. These results indicate that in a correct description of the defect-induced lattice distortion at 450 K the proper *time scale* for the defect motion should be included. The difference between the cases "$m=m_{\mathrm{Nb}}$" and "static" implies that including the thermal motion only by adding a Debye-Waller factor leads to a rather crude description of the actual q dependence of the scattering cross section.

We have also performed the same study at 300 K. At this temperature the diffusion constant for deuterium is reduced to $D_s=0.88\times10^{-5}$ cm^2 s^{-1}, which can be compared with the experimental number which is equal to $D_s=0.38\times10^{-5}$ cm^2 s^{-1}.[3] The result is shown in Fig. 3. The cases "$m=m_D$" and "$m=m_{\mathrm{Nb}}$" are now more close to each other and at this temperature the actual *time scale* for the defect motion seems to play a minor role. Still we find a difference between the cases "$m=m_D$" and "static."

Finally we would like to compare our results with the experimental findings. The absolute intensities of the diffuse scattering cross section have been measured at two different temperatures 300 K and 480 K.[7] The presented data do not contain the Debye-Waller factors e^{-2L} and e^{-2M}. To compare with our data we have therefore multiplied the experimental values with e^{-2M}, where $M=\frac{1}{2}q^2\langle u_{\mathrm{Nb}}^2\rangle$ and $\langle u_{\mathrm{Nb}}^2\rangle=5.8\times10^{-3}$ Å^2 at 300 K and $\langle u_{\mathrm{Nb}}^2\rangle=9.3\times10^{-3}$ Å^2 at 480 K.[17] The factor e^{-2L} can be neglected. The data are divided by $c_Db^2=8.57$ mb ($c_D=0.017$) and the results are given in Fig. 4.

In comparison with the observed values for $S_{\mathrm{dif}}(q)$ our data differ substantially in absolute intensities. However, the shape of the diffuse scattering function is reproduced quite well by our data, particularly at the higher temperature. There are several possible reasons for this difference in absolute intensities: (i) Our model for the Nb-Nb potential is rather crude. The phonon spectrum is not accurately reproduced but, on the other hand, our data for $S_{\mathrm{dif}}(q)$, based on Eq. (1), are quite similar to the data in Ref. 7, where a more accurate phonon spectrum has been used in a corresponding calculation. In our case anharmonicity is included but it is difficult to state to what extent that influences the result. An
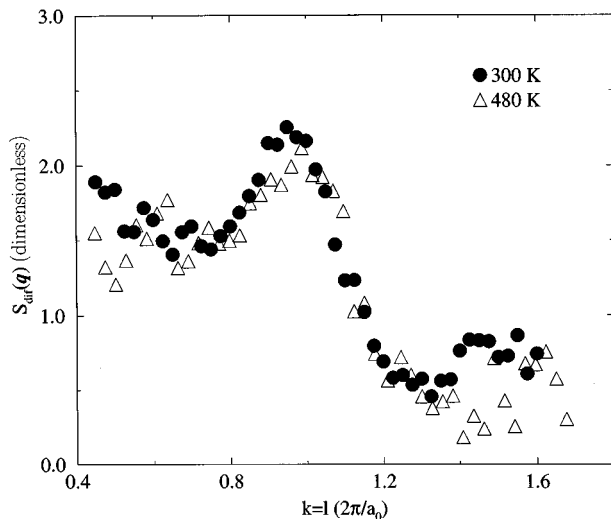
FIG. 4. Experimental values for $S_{\mathrm{dif}}(q)$ along scan 1 ($h = 3.62$) at two different temperatures, taken from Ref. 7.

important issue is how accurate our model for the interatomic interaction describes the anharmonicity in the real system. The H-Nb interaction, fitted to the first-principles calculations by Elsässer et al.,[4] is probably quite accurate but uncertainties are introduced when the assumption of a pair potential is introduced and when quantum effects are neglected in developing the model potential (cf. the discussion in Ref. 9). (ii) The scans we have used [Eqs. (3) and (4)] are not identical to the experimental scans in Ref. 7. However, this rather small change cannot explain the large difference in absolute intensities. This has been verified by calculating $S_{\mathrm{dif}}(q)$ at some other nearby positions in reciprocal space. (iii) We treat the motion of the defect classically. Based on the study in Ref. 9 the deuterium atom should be rather localized in space at the present temperature. The details of the distribution of the deuterium atom are influenced by quantum effects but we expect that to have a rather small effect on $S_{\mathrm{dif}}(q)$. (iv) The intensity of the measured cross section is very weak compared with the diffuse scattering background and a careful data analysis and calibration have to be performed in order to obtain absolute intensities. For that reason one cannot rule out possible uncertainties in the experimental data but it cannot explain the large difference in absolute intensities.

The most likely reason for the discrepancy in absolute intensities is the model potential we are using. Better models for niobium have been developed[18] but these are considerably more complicated and extensive time-dependent calculations cannot be performed as easily. Also the problem of introducing hydrogen into that model is still present. In the future it would be highly desirable to use better model potentials.

V. CONCLUSIONS

We have determined the diffuse scattering function $S_{\mathrm{dif}}(q)$ from a time-dependent calculation at finite temperatures in a way that closely resembles the experimental procedure. Two different temperatures are considered, 450 K and 300 K, and classical mechanics is assumed for the motion of the atoms. At the higher temperature it has been shown previously that our model for H in Nb describes accurately the details of the diffusive motion of hydrogen.[8,9]

We find that the usual way of introducing the thermal motion of the atoms into the expression for the diffuse scattering function through a Debye-Waller factor [cf. Eq. (1)] gives a rather imprecise description of the q dependence of the scattering cross section. In a detailed analysis of experimental data an improved description should be used.

We also find some evidence for the fact that the actual *time scale* for the defect motion influences the shape of the diffuse scattering function at 450 K. At the lower temperature 300 K, this effect seems to be of minor importance.

The obtained results for $S_{\mathrm{dif}}(q)$ are found to deviate from the experimental results in magnitude but not in shape (the q dependence). We argue that the most likely reason for this discrepancy is an inaccurate model potential.

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