Slowing down of atoms in metals studied by the Doppler-broadened γ-ray line shapes produced after thermal-neutron capture in Fe and Cr crystals

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(Received 7 December 1998)

Molecular-dynamics simulations describing the slowing down of atoms in solids are used to study interatomic potentials in metals. This analysis is achieved by observing the fine structures of Doppler-broadened γ rays emitted by the recoiling excited nuclei. The recoil of the atom, ~400 eV kinetic energy, is generated by the emission of a preceding γ ray following thermal-neutron capture. The experiment was performed with oriented single crystals of Fe and Cr as target and high-resolution γ-ray spectroscopy. Two different nuclear levels for each element were studied and the best interatomic potential among many available in the literature could be deduced from the data. The construction of a different potential was also investigated with this technique. Lifetime values with a much improved precision were obtained for four excited nuclear levels. [S0163-1829(99)01133-9]

I. INTRODUCTION

The γ-ray induced Doppler-broadening method using single crystals as target (Crystal-GRID method[1]), is based on the observation of Doppler shifts produced by the motion of emitting nuclei in a solid-state target. The recoil of the atom is generated by the emission of the excited nucleus of a primary γ ray following thermal-neutron capture. The Doppler-broadened γ-ray line shape is measured by the double-axis flat-crystal spectrometer GAMS4,[2] installed at the high-flux nuclear reactor of the Institute Laue Langevin in France. This spectrometer has an energy resolution $\Delta E/E$ of $10^{-4}-10^{-6}$ and allows one to measure small Doppler broadening. This technique is used here to study interatomic potentials in metals and to deduce short lifetimes of nuclear states. This method (see Refs. 1, 3, 4, and 5), combined with molecular-dynamics simulations, gives information on the slowing down of atoms in the bulk of materials at kinetic energies below 400 eV. Two natural isotopes (^{56}Fe and ^{53}Cr) were analyzed via four different nuclear levels populated after thermal-neutron capture. For each element, two different targets placed inside the nuclear reactor with the [100] and the [110] direction towards the GAMS4 spectrometer, were investigated.

In the literature, there exists a multitude of potentials for metals which tends to reproduce with more or less success the slowing down and motion of atoms in the bulk. However, most of these potentials, especially the embedded-atom-method (EAM) potentials, which reproduce quite well equilibrium properties such as lattice constants, cohesive energy, elastic constants etc., were never tested in the energy region of 20–400 eV due to the lack of experimental data. As the GRID method deals with these low kinetic energies and the energy loss due to free electrons can be neglected because the electronic stopping power cross section is more than two orders of magnitude lower than the nuclear stopping power for the elements studied,[6] the Crystal-GRID technique opens up an energy domain in which interatomic potentials and atomic collisions can be analyzed. A new potential was also derived for both metals using the Crystal-GRID data and molecular-dynamics simulations. This work takes into account several artifacts encountered, like correlation between two γ rays emitted in cascade and side-feeding problems. Four nuclear state lifetimes (two in ^{57}Fe and two in ^{54}Cr) were determined with the Crystal-GRID method. Because the experimental procedure and analysis is analogous to the one presented in Ref. 5, the interested reader might want to consult this work before proceeding.

II. ANALYSIS AND MOLECULAR-DYNAMICS (MD) SIMULATIONS

The Doppler-broadened γ-ray line-shape analysis requires the knowledge of the slowing down of atoms in the crystal as the Doppler shift depends on the velocity of the atom at the time of emission of the gamma ray. The MD programs simulate this by solving the Newtonian equation of motions for the positions and velocities of all atoms in a MD cell comprising between 1000 and 1500 atoms. Two MD programs were elaborated:[5] one for the equilibration of the MD cell at a temperature corresponding to the target temperature under the present irradiation conditions, and one for the calculation and storage of the recoil trajectories and velocities induced by the primary γ ray after the neutron capture reaction. After thermal equilibrium is reached in the MD cell, the velocity distribution of the atoms can be described by a Maxwell Bolzmann distribution. The second MD program gives a recoil velocity to the most central atom and follows the trajectory of the recoiling atom during a given time interval. The recoil energy (E_r) and the velocity (v_r) at the emission time of the first γ ray are, following the conservation of momentum, given by

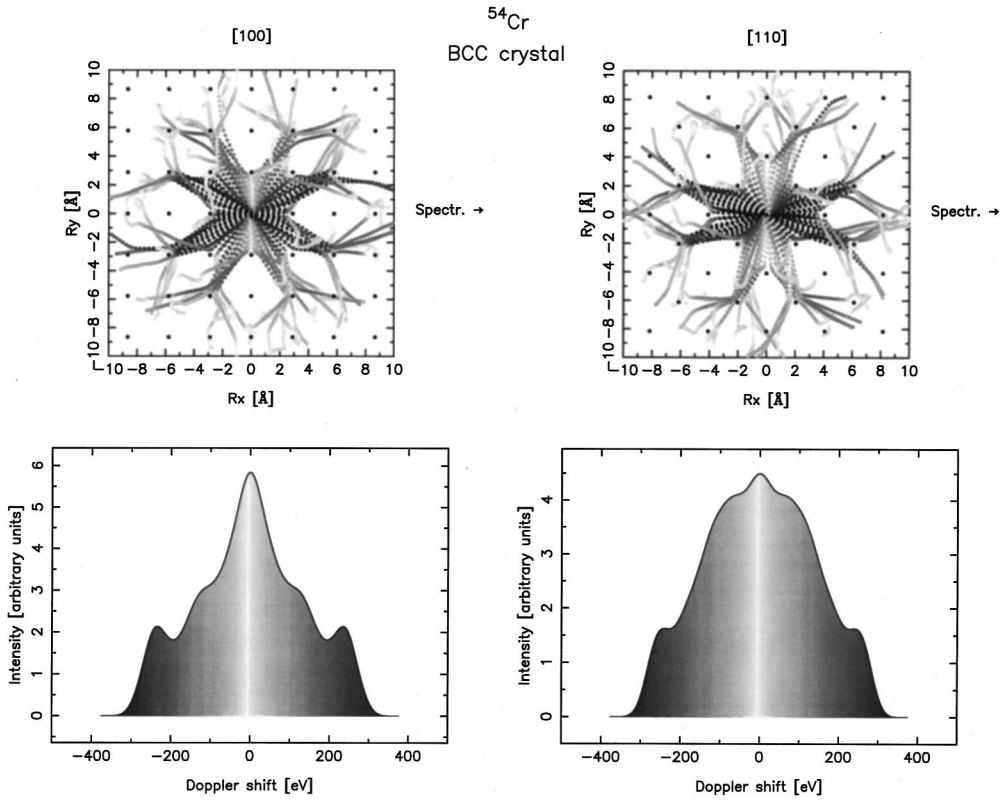

FIG. 1. Two-dimensional restricted trajectories of 100 recoils in the Cr crystal in the plane containing the direction of observation indicated by the spectrometer arrow. Each point represents the position of the recoiling atom at a time interval of 1 fs. The black point represent the position of the neighboring atoms at the beginning of the simulation. The color represents the Doppler shift (white correspond to the smallest Doppler shift, black to the greatest). The lower part represents the reconstructed simulated line shape for 1500 trajectories in three-dimensional space for a lifetime of 15.0 fs and an instrumental response approximated by a Gaussian having a full width at half maximum of 20 eV.

$$E_r = \frac{E_{\gamma_1}^2}{2Mc^2} \quad \text{and} \quad \frac{v_r}{c} = \frac{E_{\gamma_1}}{Mc^2} \tag{1}$$

with $E_{\gamma 1}$ being the energy of the first γ ray given by the difference in energy between the capture state and the populated nuclear level, M is the mass of the recoiling atom, and c is the velocity of light. The direction of the recoiling atom is randomly chosen in an isotropic way, since no preferential direction is observed for the γ-ray emission.

To reconstruct the Doppler broadened line shape from the trajectories and velocities given by the MD simulation, the scalar product between the velocity vector and the direction of observation (given by the direction of the spectrometer) is calculated. This gives the Doppler-shifted energy of the second emitted γ ray. Then the summation over all trajectories weighted by the number of γ rays emitted at that particular time will result in the line profile. The probability of γ emission is given by the exponential decay law assuming a lifetime value for the excited nuclear state populated. The Doppler-broadened γ-ray line shape is given by the following equation:

$$I(E) = C \sum_i \int_0^\infty e^{-t/\tau} \delta \left[E - E_\gamma \left(1 + \frac{v_i(t) \cdot \mathbf{n}}{c} \right) \right] dt, \tag{2}$$

where C is a normalization constant, τ is the excited nuclear state lifetime, E_γ is the nonshifted energy of the transition, $v_i(t)$ is the velocity vector of the ith simulated atom at the moment of emission as calculated by the MD programs, $\mathbf{n}$ is the relative direction of observation and c is the velocity of light. The index (i) ranges generally from 1 to 1500 and represents the number of recoil events calculated by the molecular-dynamics simulations. Figure 1 shows for chromium the simulated trajectories and simulated line shape obtained for two different crystal orientations and for a lifetime value of 15 fs. The convolution of the line profile with a Gaussian-type instrumental-response function was realized. The full width at half maximum of the Gaussian corresponds closely to the experimental function, which can be measured separately during the experiment.[2] The simulated line shape is then fitted to the measured Doppler-broadened line profile leaving the lifetime as free parameter with the least-squares fitting program GRIDDLE.[7] The fitting procedure returns a lifetime value (τ) and a χ^2 per degree of freedom which stands for the agreement/disagreement between the two line profiles. A perfect match between the two Doppler-broadened line shapes should return a value of 1.

Many interatomic potentials can be implemented in the in-house developed FORTRAN codes to check their influence on the line structure and the fitted lifetime. Roughly a decade ago, a type of potentials called the embedded-atom-method potential (EAM) was developed.[8] These interatomic potentials are based on the assumption that metallic atoms can be considered as embedded in an electron density caused by all

TABLE I. Interatomic potentials references.

Potential name	Authors	Ref.
Fe-Fe interaction		
BM	Born and Mayer	19
ZBL	Ziegler, Biersack, Littmark	16
OP	Ogorodnikow, Pokropivny	20
OMS	Osetsky, Mikhin, Serra	12
RAJ	R. A. Johnson	21
EAMVC	Voter and Chen	13
EAMGA	Guellil and Adams	22
EAMPFS	Pasianot, Farkas, Savino	23
EAMBSS	Bhuiyan, Silbert, Stott	24
Cr-Cr interaction		
BM	Born and Mayer	19
ZBI	Ziegler, Biersack, Littmark	16
OP	Ogorodnikow, Pokropivny	20
EAMGA	Guellil and Adams	22
EAMPFS	Pasianot, Farkas, Savino	23
EAMBSS	Bhuiyan, Silbert, Stott	24
EAMWB	Wang and Boerker	25

the other atoms in a crystal due to the way free electrons behave in metal. The energy of such a system is given by a summation of two terms:

$$U=\sum_i F_i(\rho_i)+\frac{1}{2}\sum_{i\neq j}\Phi_{ij}(r_{ij}), \tag{3}$$

where F_i is the energy required to embed atom i in the background electron density and Φ_{ij} is the short-range pair interaction representing the core-core repulsion between atom i and j with interatomic separation r_{ij}. The host electron density ρ_i at the position of atom i is approximated by the superposition of the atomic electron density ρ_j^a of the neighbors j by

$$\rho_i=\sum_j \rho_j^a(r_{ij}). \tag{4}$$

The two MD programs developed are based on pair potentials only and the EAM potentials need an approximation in order to avoid a double summation and long computing times. The approximation replaces the electron density ρ_i by an average electron density. A Taylor expansion over this average electron density is then realized for the evaluation of the embedding function and the interatomic potential as a function of the distance between two atoms.[9] A more detailed description of the approximation can be found in Ref. 5.

Many forms and functions, needed to calculate the interatomic potential, can be found in the literature. Table I gives a list of all the potentials (usual slowing down theories as well as EAM theories) used in this analysis for both iron and chromium. As the Born-Mayer (BM) and Ziegler-Biersack-Littmark (ZBL) potentials are only repulsive, a Morse potential[10] was added to them with a spline function to make the connection.[5] Two EAM potentials [EAMWB (Wang-Boerker), EAMPFS (Pasianot-Farkus-Savino)] used for chromium are connected to an exponential-type function (Ae^{-Br}) as the repulsive parts of the potential were insufficient to give reasonable values. The A and B values of the added exponential function are equal to 3606 eV and 0.17882 Å^{-1}, respectively. The value of A and B were chosen in order to maintain the equilibrium form of these two potentials. Figure 2 shows all potentials as a function of the interatomic distances for the two metals studied in this work.

III. DATA ANALYSIS AND RESULTS

Details concerning the experimental setup and procedure to deduce the Doppler-broadened line profile and the lifetime of excited nuclear states with the Crystal-GRID technique can be found in Ref. 5.

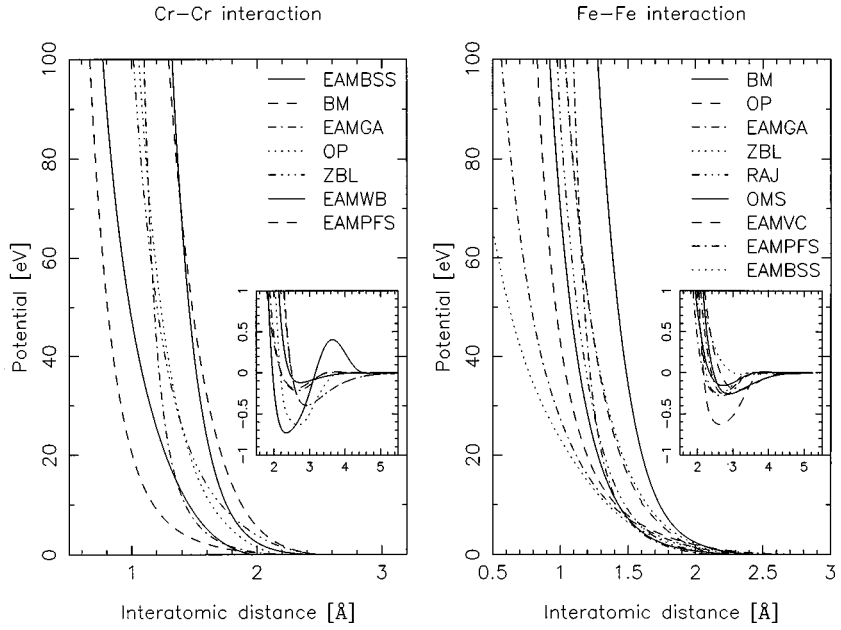

FIG. 2. Theoretical interatomic potential for the Fe-Fe (right) and the Cr-Cr (left) interaction. The potentials are placed from the most to the least repulsive potential.

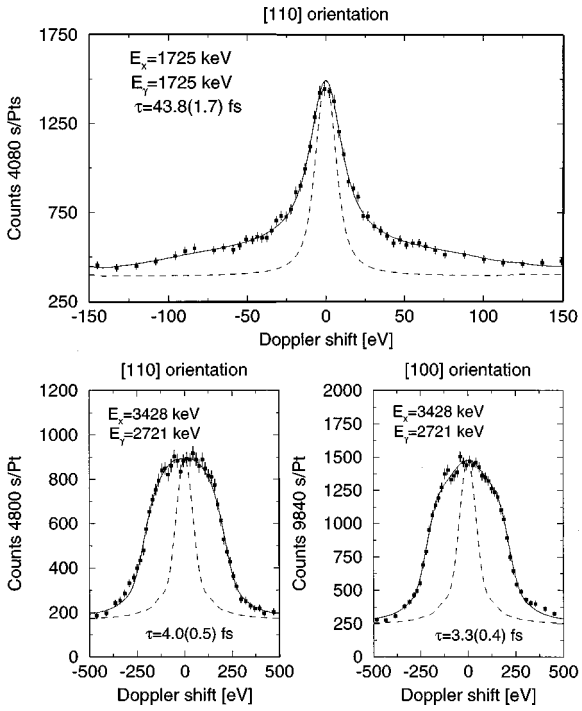

FIG. 3. Doppler-broadened γ-ray line shape of the 1725 (upper part) and 2721 keV (lower part) transition in the different orientations for the ^{57}Fe isotope. The dotted line represents the instrumental response and the full line the fitted line shape obtained with the OMS potential. The experimental line shapes are obtained by a summation of 27 (1, -1) individual scans for the 2721 keV transition in the [110] orientation, a summation of 41 (1, -1) individual scans for the 2721 keV transition in the [100] orientation, and a summation of 25 (2, -2) individual scans for the 1725 keV transition.

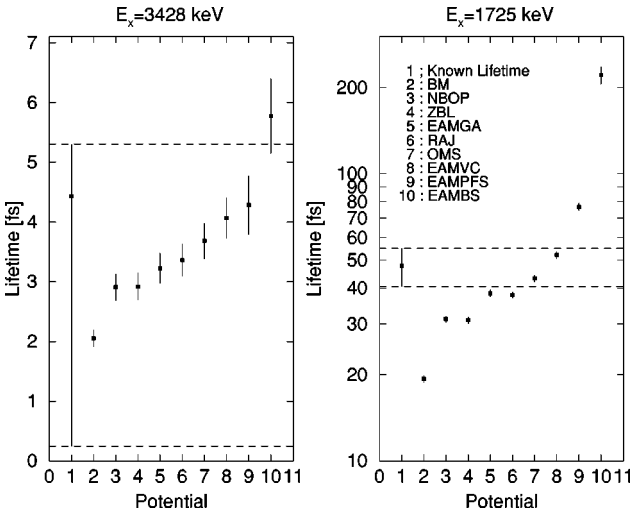

FIG. 4. Lifetime value for both nuclear levels in ^{57}Fe obtained with the MD simulation by fitting the calculated line profile to the GAMS4 data. Also shown is the known lifetime and its range found in the literature.

A. Fe experiment

The analysis is realized with two excited nuclear levels at 3428 and at 1725 keV. The Doppler-broadened γ-ray line shapes associated with the two nuclear levels and measured by the GAMS4 spectrometer are shown in Fig. 3. The lower part shows the γ-ray line shape of the 2721 keV transition for both orientations. As it can be seen, the line profile differs for a given direction of observation due to the crystalline structure of the target. The change in the line profile is, however, not very large, because, as the nuclear state lifetime is

TABLE II. The ^{57}Fe nuclear state lifetimes obtained with different potentials using the MD simulations fitted to the GAMS4 data. The χ^2 value is the summation of all the absolute χ^2 divided by the number of degree of freedom.

Potential name	E_x (keV)	E_γ (keV)	Lifetime both orientations (fs)	χ^2 both orientations	$\Sigma\chi^2$ both orientations both levels
BM	3427.67	2721.17	2.0(0.1)	1.1298	
	1725.38	1725.29	18.3(0.5)	1.0691	1.1033
ZBL	3427.67	2721.17	2.8(0.2)	1.1292	
	1725.38	1725.29	30.9(0.8)	1.0725	1.1045
OP	3427.67	2721.17	2.8(0.2)	1.1292	
	1725.38	1725.29	31.2(0.8)	1.0690	1.1030
RAJ	3427.67	2721.17	3.3(0.3)	1.1291	
	1725.38	1725.29	37.8(1.0)	1.0684	1.1027
OMS	3427.67	2721.17	3.6(0.3)	1.1291	
	1725.38	1725.29	43.2(1.1)	1.0692	1.1030
EAMBSS	3427.67	2721.17	5.7(0.6)	1.1281	
	1725.38	1725.29	220(15)	1.1213	1.1251
EAMGA	3427.67	2721.17	3.6(0.3)	1.1301	
	1725.38	1725.29	38.3(1.1)	1.0707	1.1042
EAMVC	3427.67	2721.17	4.0(0.3)	1.1288	
	1725.38	1725.29	52.1(1.4)	1.0738	1.1048
EAMPFS	3427.67	2721.17	4.2(0.4)	1.1282	
	1725.38	1725.29	76.7(2.2)	1.0940	1.1133

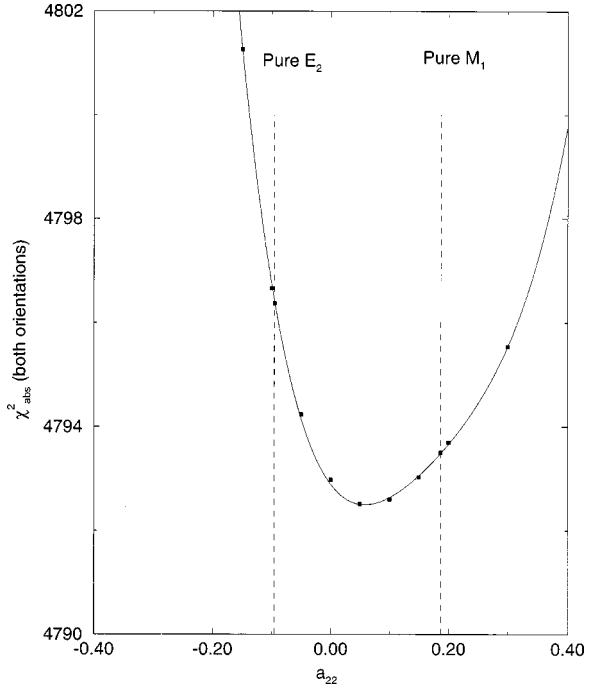

FIG. 5. Absolute χ^2 versus the a_{22} coefficient of the angular correlation for the EAMVC potential. The absolute χ^2 is obtained by a summation of the absolute χ^2 from both [100] and [110] orientations for the 3428 keV transition. The number of degree of freedom for the [100] and [110] orientation are equal to 1664 and 2582, respectively.

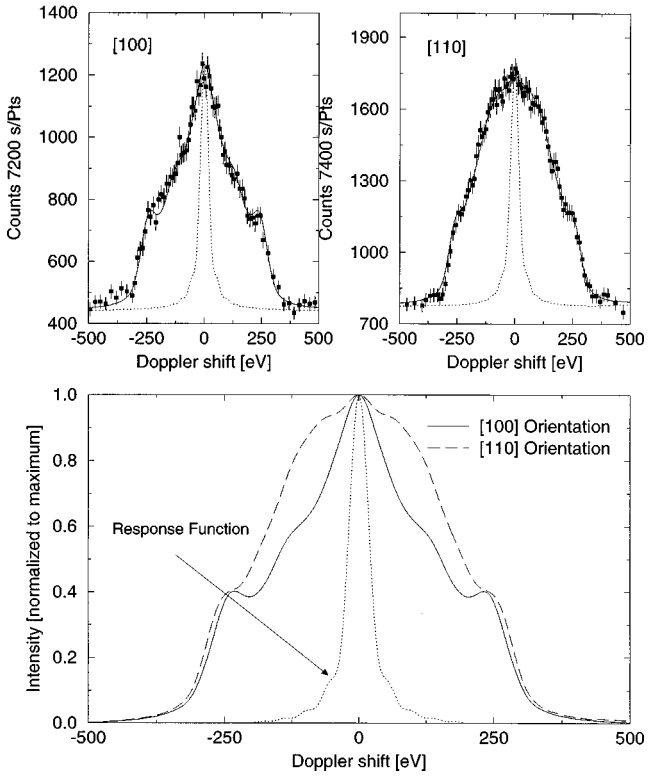

FIG. 6. The γ-ray line shape of the 2239 keV transition in the [100] and [110] orientation. The dotted line represents the instrumental response and the full line the fitted line shape obtained with the EAMWB potential. The experimental line shapes are obtained from a summation of 36 and 37 individual scans for the [100] and [111] orientation, respectively. The lower part shows the fitted line shape for both orientation with the maximum intensity normalized to 1.0.

short (~4 fs), the nucleus did not change much its direction due to collisions with neighboring atoms, before it emits the second γ ray. The blocking and channeling of the atom is therefore less visible. The selection of the best potential among a list of nine is first made by comparing the lifetime value. Table II gives the lifetime values and the χ^2 per degree of freedom obtained by the Crystal-GRID method. Figure 4 shows the different lifetime values obtained by fitting the line shape calculated by the MD simulations to the measured GAMS4 data. Also shown in this figure is the lifetime found in the literature with its error range.[11] As Fig. 4 shows, only two potentials are able to reproduce the adopted literature lifetime, namely the Osetsky-Mikhin-Serra[12] (OMS) and EAM–Voter-Chen[13] (EAMVC) potential. All the others are either too or not enough repulsive in order to explain the slowing down of atoms in the iron metal. The second criterion for the selection of the best potential is the χ^2 per degree of freedom. The OMS potential gives an overall value closer to one, which indicates that this potential is our best candidate considering the lifetime and χ^2 values (see the last column of Table II). By comparing the χ^2 for the two transitions and for the two slowing down theories (see column 5 of Table II), we can conclude that the OMS potential is the best for high energy, and the EAMVC is more suited for low energy, as the two γ rays cascade including the transition from the capture state to the 1725 keV nuclear level and then the 1725 keV γ-ray transition results in a higher recoil energy [see Eq. (1)] for the emitting atom because the first transition is of higher energy. The lifetime value obtained by the Crystal-GRID technique is by far more precise than the value found in the literature. The EAMVC, which is the best slowing down theory based on the embedded-atom method, returns a lifetime of 4.0(0.9) fs for the 3428 keV nuclear state and of 52(1) fs for the 1725 keV nuclear state in the ^{57}Fe isotope. The error includes all instrumental uncertainties. The EAMVC slowing-down theory is, according to the Crystal-GRID analysis, one of the best potentials to reproduce the motion of atoms in a crystal. The same conclusion about this potential was obtained with the Ni analysis of Ref. 5. As this potential was first designed to give equilibrium properties,[13] we can now conclude that this EAM potential is also suited in the 0–500 eV energy range. The Crystal-GRID analysis has, however, demonstrated that, although many EAM potentials are able to reproduce quite well the equilibrium properties, there are in general not all good candidates for the slowing down of atoms in metal for higher energies.

As can be seen in Table II, the lifetime value obtained for the 3428 keV nuclear level is very short (2–6 fs). In this particular case, an angular correlation between the first and the second γ ray might influence the Doppler-broadened line structure, because the direction of emission of two γ rays, which are subsequently emitted in a cascade, is correlated.[4] The unequal population of the magnetic substates of each level in the γ cascade is responsible for the angular distribution of the second γ rays with respect to the direction of the first one. This distribution depends on several factors like (i) the parity and spins of the nuclear levels, (ii) the lifetime of

the intermediate nuclear state, and (iii) the mixing ratio of the transitions involved. If very short lifetimes are measured, the correlation is observable as the nucleus did not have time to make collisions and did not change much its direction. With the characteristics of the nuclear level and transition used in the ^{57}Fe isotopes, the correlation between the two γ rays emitted in cascade, can be observed. However, for this particular isotope, the multipolarity of the second transition is not known.[11] The directional correlation $W(\theta)$ between the first and second γ ray emitted is given by

$$W(\theta)=1+a_{22}P_2(\cos\theta)+\cdots+a_{k_{\max}k_{\max}}P_{k_{\max}}(\cos\theta) \tag{5}$$

with $P_k(\cos\theta)$ the Legendre polynom of degree k. In the case of ^{57}Fe and the transitions involved, the a_{22} value is the only parameter needed to explain the distribution of the direction,[14] because $k_{\max}$, which is equal to the minimum of $2I_b,2L_1,2L_2$ (I_b being the spin of the intermediate level, L_1 and L_2 the multipolarity of the first and second transition, respectively), takes a value of 2 as L_1 is a pure $E1$ transition[11] between the $1/2^+$ capture state and the $3/2^-$ excited nuclear level at 3428 keV. As the intermediate nuclear level has a $3/2^-$ spin and the final a spin of $5/2^-$, the multipolarity of the transition is pure $M1$, pure $E2$ or a mixing between the two. The first analysis compares the χ^2 obtained by fitted the simulated line shape to the measured line profile with the most extreme a_{22} parameters, which are obtained when the second transition is considered to be a pure $M1$ or $E2$ transition. The preferential direction of emission of the second γ ray versus the first emitted γ ray due to angular correlation is included in the simulation program. The direction of the recoil is chosen randomly with a distribution given by the Legendre polynoms associated with the mentioned a_{22} coefficient. Taken into account all the slowing down theories mentioned (see Table I) and all the data measured for iron, we found that the 2721 keV transition multipolarity $M1$ ($a_{22}=0.1871$) returns a better χ^2 per degree of freedom in 64% of the cases than the $E2$ ($a_{22}=-0.09545$) multipolarity. A second a_{22} analysis was realized by taking a_{22} values in-between the most extreme parameters assuming that the second transition can be a mixing between a $M1$ and $E2$ transition. Figure 5 shows the behavior of the χ^2 versus the a_{22} value for the EAMVC interatomic potential. This fit returns a a_{22} value of $0.06^{+0.13}_{-0.09}$, with a 1σ error. Both analyses indicate that the transition is probably a mixing between an $M1$ and $E2$ with a slightly higher percentage for the $M1$ character. Taking into account the possible angular correlation error and the instrumental response uncertainties, the Crystal-GRID method returns a value of $4.0^{+2.6}_{-1.7}$ fs for the 3428 keV nuclear state lifetime.

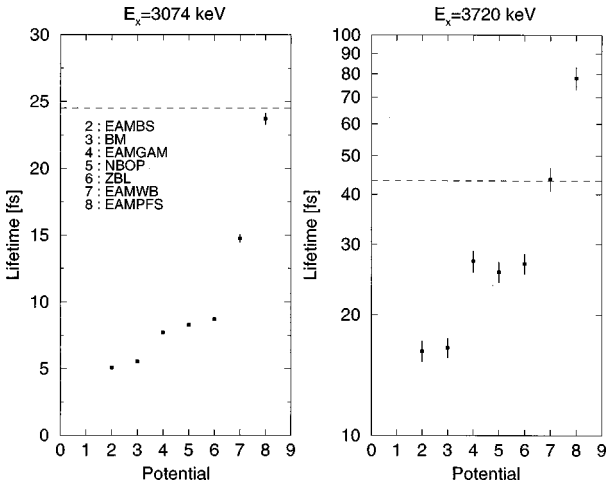

FIG. 7. Lifetime value for both nuclear levels in ^{54}Cr obtained with the MD simulation by fitted the calculated line profile to the GAMS4 data. Also shown in the known lifetime and its range found in the literature.

The second 1725 keV excited nuclear state has another

TABLE III. The ^{54}Cr nuclear state lifetimes obtained with different potentials using the MD simulations fitted to the GAMS4 data. The χ^2 value is the summation of all the absolute χ^2 divided by the number of degree of freedom.

Potential name	E_x (keV)	E_γ (keV)	Lifetime both orientations (fs)	$\Sigma\chi^2$ both orientations	$\Sigma\chi^2$ both orientations both levels
BM	3073.94	2239.07	5.6(0.1)	1.1098	
	3719.88	3719.88	16.6(1.0)	1.0854	1.0876
OP	3073.94	2239.07	8.3(0.1)	1.1110	
	3719.88	3719.88	25.6(1.5)	1.0840	1.0864
ZBL	3073.94	2239.07	8.7(0.2)	1.1108	
	3719.88	3719.88	26.8(1.6)	1.0835	1.0859
EAMBSS	3073.94	2239.07	5.1(0.1)	1.1120	
	3719.88	3719.88	16.2(1.0)	1.0953	1.0968
EAMGA	3073.94	2239.07	7.7(0.1)	1.1102	
	3719.88	3719.88	27.2(1.7)	1.0901	1.0918
EAMWB	3073.94	2239.07	14.8(0.3)	1.1075	
	3719.88	3719.88	43.7(3.0)	1.0793	1.0817
EAMPFS	3073.94	2239.07	23.7(0.5)	1.1075	
	3719.88	3719.88	78.9(5.1)	1.0804	1.0828

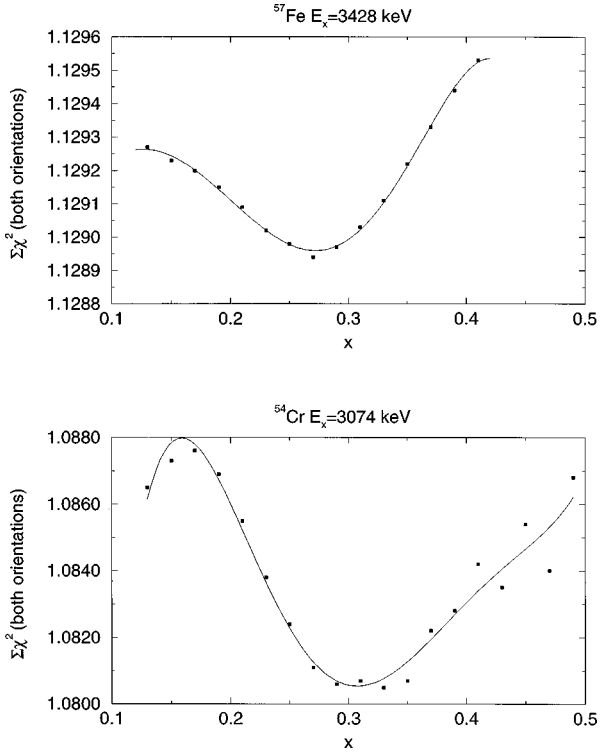

FIG. 8. χ^2 per degree of freedom versus the x parameter of the ZBL potential for iron and chromium. The χ^2 is obtained by a summation of the absolute χ^2 of both orientations divided by the total number of degrees of freedom. The full line represents a fifth-order polynomial fit.

particularity, since the level is not 100% populated by the direct feeding, which would insure a unique initial recoil energy. This leads to multiple initial recoil energies as the recoil can be induced by several side feeding transitions. The 1725 keV nuclear level is only populated by 89.2% of the cases by the direct transition from the capture state.[11] The 10.8% side feeding has however an influence of less than 5% on the nuclear lifetime deduced from the MD simulations and the GAMS4 data. The error is of the same order of magnitude as the instrumental response uncertainties measured separately. The final value obtained for the nuclear level, including the error on the instrumental response and side feeding, returns a lifetime value of 52(3) fs for the 1725 keV nuclear state with the EAMVC interatomic potential.

B. Cr experiment

The best candidate to check the difference in the line structure depending on the crystal orientation with respect to the spectrometer is the nuclear level at 3074 keV in chromium, because the lifetime is in the right order of magnitude. With this lifetime value (~15 fs), the atom has sufficient time to make a couple collisions with its neighbors before the γ ray of interest is emitted. Therefore, the channeling and blocking of the atoms due to the ordered structure in the crystal will influence greatly the form of the Doppler-broadened γ-ray line shape. Figure 6 shows the Doppler-broadened γ-ray line shape in the [100] and [110] orientation obtained with the 2239 keV transition. The difference in the line structure is obviously dependent on the crystal orientation with respect to the direction of observation. The [110] line structure is more broadened, because, when the recoiling atom moves in the [110] direction (which will give the greatest Doppler shift), it will be less slowed down than in the [100] direction due to the greater distance between nearest neighbors. The atoms' positions and nearest-neighbor distances in a bcc crystalline structure can be seen in Fig. 1.

Seven interatomic potentials were tested by the lifetime value obtained from the Crystal-GRID measurements and the χ^2 value indicating the agreement/disagreement between the simulated and measured line shape. In the chromium case, the selection of the best slowing down theory can only be made with one criterion because the lifetime for both nuclear levels are not known with sufficient precision.[15] Only an upper limit was measured by other means and almost all of the deduced lifetimes calculated with the different interatomic potentials are lower than this limit (see Fig. 7). The selection of the best potential is, therefore, realized with the χ^2 value. The best slowing down theories in term of the χ^2 is given by the EAMWB potential as Table III shows. This potential associated with the measured Doppler-broadened line shape returns a lifetime value of 14.8(0.3) fs for the 3074 keV nuclear state and a lifetime of 44(3) fs for the 3720 keV state. The error includes the instrumental uncertainties. The EAMWB is therefore a good candidate to reproduce the equilibrium properties of the metal as well as the motion of atom having a recoil energy of a few hundreds of eV. The validity of our approach could be crosschecked if the lifetimes could be determined by other means.

IV. CONSTRUCTION OF A NEW POTENTIAL

From the Crystal-GRID data, a type of potential based on the ZBL theory[16] was developed for the Fe-Fe and Cr-Cr interactions. The ZBL potential is a Coulomb-screened potential calculated with several parameters identical to all elements and with functions dependent on the charge (Z_i) of atoms in the interaction.[16] As we are dealing with atoms recoiling in the same material, only one parameter, the x parameter, can be adjusted.[5] This x parameter is taken as the free value in the equation defining the potential. By regard-

TABLE IV. Adopted lifetime values for two nuclear levels in iron and chromium.

Isotope	Nuclear level energy (keV)	Slowing down theory used	Lifetime (fs)	Lifetime Refs. 17, 18 (fs)
^{57}Fe	3427.67	EAMVC	4.0(2.6)	$4.3(^{+0.9}_{-4.2})$
	1725.38	EAMVC	52(3)	42(3)
^{54}Cr	3073.94	EAMWB	14.8(0.3)	13(2)
	3719.88	EAMWB	44(3)	31(5)

ing the χ^2 value as a function of the x parameter one can deduce the best parameter possible for the slowing down of atom in its crystal. Figure 8 shows the behavior of the χ^2 per degree of freedom in function of the x parameter for both metals. The fit returns with a 1σ confidence level an x parameter of $0.27^{+0.08}_{-0.16}$ and $0.31^{+0.02}_{-0.02}$ for iron and chromium, respectively. This value is to be compared with the 0.23 value of the original paper of ZBL.[16] These two derived potentials have the same form as the best potentials found by the regular analysis (see the OMS and EAMWB potential in Sec. III) and as such confirm our conclusions. The fitted lifetime obtained with the derived ZBL potential is equal to 3.4(0.3) fs for the 3428 keV nuclear level in ^{57}Fe and 13.1(0.3) fs for the 3074 keV nuclear level in ^{54}Cr.

V. CONCLUSION

We have analyzed by the Crystal-GRID method the slowing down of atoms in the bulk for two transition metals. The analysis is able to make a selection of the best interatomic potential among a list of several potentials and also permits the construction of a potential based on a known theory by fitting a parameter in order to reproduce the measured line shape. The analysis returns lifetime values for four nuclear states in ^{57}Fe and ^{54}Cr with a good precision. The dependence of the crystal orientation with respect to the direction of observation was demonstrated, and the analysis proves that blocking and channeling of neighboring atom due to the ordered structure in a crystal play an important role in the Doppler-broadened γ-ray line shape. Table IV gives the adopted lifetime value for the nuclear levels studied with the Crystal-GRID taking into account all possible error propagation. It should be noted that a GRID measurement using polycrystalline targets and a simple slowing down theory[4] was performed about ten years ago for Fe and Cr.[17,18] Here we did not use their results as they were not derived using a completely independent method. The lifetime values found with the analysis are, however, in good agreement with the result obtained in Ref. 17 for Fe and Ref. 18 for Cr as illustrated in Table IV.

ACKNOWLEDGMENTS

This work was supported by the Swiss National Research Fund. The authors are especially grateful to Dr. A. Voter of Los Alamos National Laboratory, to Professor M. Siebert and Dr. G. Bhuiyan, from the School of Physics, University of East Wenglia, United Kingdom, and to Professor Dr. Farkas from the Department of Materials Sciences and Engineering, Virginia Polytechnic for providing useful information and discussions on embedded-atom-method potentials.

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