Swift heavy ion irradiation of SrTiO$_3$ under grazing incidence

Ender Akcöltekin$^1$, Sevilay Akcöltekin$^1$, Orkhan Osmani$^1$, Andreas Duvenbeck$^1$, Henning Lebius$^2$ and Marika Schleberger$^{1,3}$

$^1$ Experimentelle Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany
$^2$ CIMAP, blvd. Henri Becquerel, 14070 Caen Cedex 5, France
E-mail: marika.schleberger@uni-due.de

New Journal of Physics 10 (2008) 053007 (13pp)
Received 25 January 2008
Published 7 May 2008
Online at http://www.njp.org/
doi:10.1088/1367-2630/10/5/053007

Abstract. The irradiation of SrTiO$_3$ single crystals with swift heavy ions leads to modifications of the surface. The details of the morphology of these modifications depend strongly on the angle of incidence and can be characterized by atomic force microscopy. At glancing angles, discontinuous chains of nanosized hillocks appear on the surface. From the variation of the length of the chains with the angle of incidence the latent track radius can be determined. This radius is material specific and allows the calculation of the electron–phonon coupling constant for SrTiO$_3$. We show that a theoretical description of the nanodot creation is possible within a two-temperature model if the spatial electron density is taken into account. The appearance of discontinuous features can be explained easily within this model, but it turns out that the electronic excitation dissipates on a femtosecond timescale, too rapidly to feed sufficient energy into the phonon system in order to induce a thermal melting process. We demonstrate that this can be solved if a temperature-dependent diffusion coefficient is introduced into the model.
1. Introduction

The irradiation of solid matter with heavy ions of 100 MeV energy has long been known to create structural modifications ranging from defects and amorphization in the bulk up to the creation of hillocks on the surface [1]–[4].

In this energy range, the projectile is slowed down almost exclusively by electronic interactions. The standard model to describe the energy transport is based on a two-temperature model and includes solving the heat diffusion equation in a cylindrical symmetry [5]–[7]. This approach requires many approximations as well as the fitting of the strength of the electron–phonon coupling. The model has been quite successful in explaining, e.g. track radii in various materials created by irradiation perpendicular with respect to the surface [6].

If the sample is irradiated under grazing incidence, it has recently been shown that chains of nanodots can be created by single ions [8, 9]. In an earlier experiment, similar elongated tracks on a LiF surface covered with gold particles have been observed and were explained in terms of an elastic shock wave model [10]. These phenomena can no longer be described by the conventional thermal spike model for several reasons. First of all, the cylindrical symmetry is no longer given. More important, the electron density cannot be approximated by a homogeneous electron gas because the electronic structure plays a major role in the creation of the chains.

To explain these striking experimental findings and to overcome the limitations of the conventional approach a model was proposed where the creation of hillocks is directly coupled to the spatial electron density of the material [8]. Every time the projectile travels through a region with a high density the energy loss is sufficiently high to feed energy into the electronic system. This electronic excitation energy is then transported out of the excitation zone due to electron–electron scattering and may reach the surface. Subsequently, energy is transferred from the electronic to the nuclear system via electron–phonon coupling. Due to this localized heating the melting temperature is reached only in a confined volume. If this melting process happens close enough to the surface a nanodot (of as yet unknown structure) appears on the surface. Since the electron density corresponds to the periodicity of the crystal the nanodots appear on the surface with a certain periodicity depending on the exact impact parameters. Note that the creation of holes, which plays a significant role in the case of insulators and has been discussed in detail by Klaumünzer [11] is not taken into account in the current version of our approach.

The aim of this paper is to study the track creation in SrTiO$_3$ in more detail. We extend the model proposed by Akcöltekin et al [8] in order to determine the electron–phonon coupling constant and to study the diffusion of energy within the electron and the phonon system.
Figure 1. Left panel: AFM image of a clean SrTiO$_3$(100) surface taken in situ, roughness is rms < 1 nm. Frame size is 800×800 nm$^2$. Right panel: surface after irradiation with 130 MeV Pb ions, $\Theta = 90^\circ$, fluence $1 \times 10^9$ ions cm$^{-2}$. Inset shows a three-dimensional image of a single hillock which has a height of 4.5 nm. Image size is 2×2 $\mu$m$^2$.

2. Experimental procedures

Single crystal samples of SrTiO$_3$(100) and SrTiO$_3$(111) (Crystec, Berlin) have been irradiated without prior surface treatment at the ion beam facility IRRSUD of the GANIL, France. The irradiation was done using $^{207}$Pb$^{28+}$ and $^{131}$Xe$^{23+}$ ions with kinetic energies of 130 and 93 MeV, respectively. These charge states are close to the respective equilibrium charge states [12]. The charge state effects on the stopping power are, therefore, neglected in the present paper. Thus, the energies correspond to stopping powers of 22 and 19 keV nm$^{-1}$, respectively, as calculated with SRIM [13]. The angle of incidence with respect to the surface was varied between $\Theta = 90^\circ$ and 0.3$^\circ$. Fluences were typically chosen to yield between 5 and 20 impacts per $\mu$m$^2$. After irradiation the samples were analyzed by atomic force microscopy (AFM) either in the intermittent contact mode under ambient conditions or in contact mode in UHV. All AFM images were processed with the Nanotec Electronica SL WSxM software, version 4.0 Develop 8.3. [14]. From the raw data (400×400 data points) only a plane was subtracted. The color code was changed using the palette flow.lut. No change of contrast (1) or brightness (0) was used.

3. Experimental results

Since the samples undergo no surface treatment prior to irradiation, we make sure that the virgin surface is sufficiently characterized to be able to identify modifications due to irradiation. In the left part of figure 1 a typical AFM image of an untreated SrTiO$_3$ surface is shown. The irregular step edges separating the terraces can be clearly seen. The average step height is about $(3 \pm 0.5)$ Å, this is in reasonable agreement with the literature value of 3.905 Å [15]. The surface roughness is rms $\lesssim$ 1 nm.

After irradiation at $\Theta = 90^\circ$ nanosized hillocks have appeared on the otherwise unchanged surface. The sample shown in the right part of figure 1 was exposed to a fluence of $1 \times 10^9$ ions cm$^{-2}$. On average, we find 11 hillocks per square micron on this surface, i.e. every ion impact produces one of these nanodots.

If we change the angle of incidence from $\Theta = 90^\circ$ down to angles of 10$^\circ$, the shape of the hillocks remains unchanged. However, if the angle is decreased even further the morphology of the irradiation induced damage changes drastically. This can be seen from figure 2. This series
Figure 2. AFM images of SrTiO$_3$ surfaces irradiated with 96 MeV Xe ions. Upper row, from left to right: angle of incidence 6°, 5° and 4°. Lower row, from left to right: angle of incidence 3°, 2° and 1°. Image size is 1.2 × 1.2 µm$^2$, scale runs from 0 nm (blue) to 5 nm (orange). White arrows indicate direction of irradiation. Line scans are taken from highlighted regions.
Figure 3. Length distribution for two different angles of incidence (θ = 5° and 0.5°) determined from 105 and 60 individual tracks, respectively. Binning interval 10 and 200 nm, respectively.

of AFM images demonstrates that the hillocks at first elongate along the direction of the ion trajectory (indicated by arrows), then elongated structures with two or three separate maxima appear, and finally chains of totally disconnected hillocks are created. Again, the number of chains corresponds to the fluence, so that each ion creates one chain. These chains can have a total length of a few microns, contain dozens of nanodots and these nanodots seem to exhibit a certain periodicity. The dimensions of the nanodots within the chains are comparable to the dimensions determined from the θ = 90° experiment (see inset and linescans).

By comparing samples irradiated with xenon ions with those irradiated with lead ions (not shown here), no significant differences in the morphology could be detected.

4. Discussion

It is clearly apparent from figure 2 that the length of the track varies with the angle of incidence. In order to quantify this we determined the length distributions as a function of the angle of incidence by analyzing at least 60 tracks for each angle. As an example, we present the length distribution for θ = 0.5° and 5°, respectively (see figure 3). Both are slightly asymmetric, for the extremely glancing angle the distribution is centered around 750 nm whereas the mean length at 5° is 100 nm. The distribution for the glancing angles is much broader, most likely due to the limited number of analyzed chains.

The ion excites the electronic system along the track and the energy is later transferred to the lattice via electron–phonon coupling. In a region where the local energy density is high enough, defects can be created, melting and amorphization may occur. Therefore, the ions trajectory is surrounded by a modified region (track) with a radius given by d. The corresponding geometric relation describing the angle dependence has already been established in [8] and is applied here as well (see figure 4):

\[ L = d / \tan \theta, \]  

with the chain length L and d being the maximum depth (measured perpendicular to the surface) from which the excitation may reach the surface (see inset in figure 4). This simple model
assumes that a part of the latent track in the volume can be detected at the surface as a chain of hillocks.

How far the local excitation can spread (i.e. the value of $d$) depends entirely on the material properties, such as the electron–phonon coupling constant, the heat capacity, the heat conductivity and the melting temperature. In a metal, e.g. it is well known that the energy dissipation within the electronic system is so fast that on a timescale necessary for the lattice to react (a few 10 ps) the local energy density is already too low to create any permanent damage. As $d$ should not depend on the different experimental conditions but only on the material, we plotted all the data (irradiations with Xe as well as Pb obtained from a (100) and a (111) surface, respectively) in a single graph. As one can see from figure 4 our data can be fitted quite well with one curve, yielding $d = 8 \text{ nm}$.

Understanding the position of the individual hillocks within the chain is more complicated and cannot be explained by this simple relation. The reason is that the spatial details of the electronic structure play an important role here. SrTiO$_3$ is an insulator and most valence electrons are located close to the oxygen atoms, a few around the titanium and almost none at the strontium sites. The energy loss of the projectile is taken to be proportional to the electron density along the track, i.e. no distant collisions are taken into account. The energy loss is thus significant only in regions where the electron density is high and the ion experiences a strongly varying force corresponding to the local variations of the electron density. We therefore follow the approach described in [8] and use the DFT electron density$^4$ to calculate the stopping power $dE/dx$ along the ion trajectory [19] according to the Lindhard stopping formalism [20].

$^4$ The DFT calculations were performed using the ABINIT package [16] together with pseudopotentials generated by the fhi98pp code [17]. For the exchange-correlation energy the Perdew–Burke–Enzerhof generalized-gradient approximation functional [18] was used. The electron density was derived at the equilibrium lattice constant ($7.53 \text{ \AA} \text{Bohr}$ for SrTiO$_3$). In all calculations a common kinetic-energy cutoff-energy of 96 Hartree for the expansion of the wavefunctions and an $8 \times 8 \times 8$ k-point mesh were used.
Figure 5. Calculated electronic stopping along different example trajectories with different $\Theta$ and $\phi$. (a): $\Theta = 0.4^\circ$ with respect to the [001] direction and $\phi$ along the [001] direction; (b): $\Theta = 0.4^\circ$ and $\phi = 10^\circ$ with respect to the [001] direction. (c): $\Theta = 0.4^\circ$ with respect to the [011] direction and $\phi$ along the [011] direction; (d): $\Theta = 0.4^\circ$ with respect to the [011] direction and $\phi = 1.0^\circ$ towards the [112] direction. The red line represents the moving average of the data, averaging width 10 nm.

results for an ion traveling almost (deviation corresponding to $\Theta = 0.4^\circ$) along the [001] and [011] directions are shown in figures 5(a) and (c), respectively.

We then calculate the moving average (averaging width 10 nm, red lines in figure 5) of this data to take into account that hillocks can only be created if the average energy density in this region is high enough. The distance between the local maxima in the averaged stopping power for typical experimental parameters is, e.g., $\approx 55$ nm (see figure 5(a)) and corresponds well with the experimentally observed distances between hillocks. However, we wish to point out that in certain geometries a slight deviation from the azimuthal angle can have a rather large influence on the exact positions of the maxima in the stopping power along the trajectory. For example, a trajectory which deviates $10^\circ$ from the [001] direction appears still very regular but with new maxima in between the old ones (see figure 5(b)). On the other hand, a trajectory deviating from the [011] direction by $1^\circ$ towards the [112] direction (see figure 5(d)) already appears very irregular. Therefore, the hillocks within the chains are usually not as equally spaced as one would probably expect. In addition, the electron excitation is a statistical process, i.e. hillocks may appear differently even along identical crystallographic trajectories.

To demonstrate the influence of the azimuthal angle more clearly we have irradiated a (100) oriented crystal surface along the [001] direction and a (111) surface along the [011] direction.
Figure 6. (a): AFM image of a track created on a SrTiO$_3$(100) surface, $\Theta = 0.5^\circ$, $\phi \approx 0^\circ$. (b): AFM image of a track created on a SrTiO$_3$(111) surface, $\Theta = 0.5^\circ$, $\phi \approx 45^\circ$. Image size is 200 $\times$ 850 nm$^2$.

(exact within a few degrees). By using crystals of different orientations it is possible to probe higher indexed directions and still use glancing incidence angles. The results are shown in figure 6. The tracks appear very similar at first but a detailed analysis reveals minor differences: on the (111) surface the nanodots tend to appear in closely neighboring pairs (figure 6(b)) whereas on the (100) surface the dots appear to be more regularly spaced (figure 6(a), compare with figure 5(a)). In fact, the chain in figure 6(a) exhibits a periodicity of $(58 \pm 8)$ nm, which corresponds to a lattice constant of 3.9 Å if we assume in our simulation that the ions hit the surface under $\Theta = 0.4^\circ$. This value is in very good agreement with the angle of irradiation of $\Theta = (0.5 \pm 0.2)^\circ$ nominally used in the experiment. The images clearly indicate that the dots represent a direct projection of the electron density onto the surface. Such a quantitative comparison of any given trajectory with the calculations is, however, not possible because the experimental parameters (i.e. polar and azimuthal angles) cannot be controlled with the required precision.

From the analysis above it is evident that electronic excitation must be the source for the creation of nanodots. However, the creation of dots requires the movement of atoms, i.e. the transfer of energy from the electronic into the phononic system. Within the two-temperature model this is implemented by introducing an electron–phonon coupling constant $g$, which controls the energy flux. As sources of excitation energy fed into the electronic subsystem, the space and time dependent energy loss along the trajectory enters the calculation. In addition, the spatial and temporal evolution of the energy density has to be calculated which is done by solving the heat diffusion equation using the finite difference method combined with Neumann boundary conditions. The calculated energy per unit volume can be used as initial conditions for a molecular dynamics simulation in order to compute the nuclear displacements. This is however, not within the scope of this paper.

Since the parameter $d$ is material specific it can be used to determine the electron–phonon coupling constant $g$ as follows: from figure 4 we can determine the track length that the ion has to travel before it can no longer create modifications on the surface. In the case of $\Theta = 0.3^\circ$ and $d = 8$ nm (see [8] and figure 4) this length would be $\approx 1530$ nm. We calculate the energy loss at the end of that trajectory and project it onto the surface. We subsequently calculate the temperature at the surface for different values of $g$. For the conversion of energy into temperature, we use the experimentally determined heat capacity of SrTiO$_3$ of $C_l = 100$ J (K mol)$^{-1}$ [21]. If we assume that in order to modify the surface, at least the melting temperature of SrTiO$_3$ ($T_{\text{melt}} = 2353$ K [15]) has to be achieved, we find that $g \approx 1 \times 10^{18}$ W (m$^3$K)$^{-1}$ as can be seen from figure 7. Experimentally determined values of $g$ for other materials are in good agreement with our finding [22, 23].

After $g$ and the source terms $B(\vec{r}, t)$ for the electronic excitation have been determined, the diffusion equations describing the energy relaxation within the two-temperature model can be
Figure 7. Temperature in K on the surface as a function of the electron–phonon coupling constant $g$. The bar on the temperature axis marks the melting temperature of SrTiO$_3$. The red line represents a linear fit to the data.

solved using finite differences and with Neumann boundary conditions. As initial temperature zero K was chosen.

$$\frac{\partial T_e}{\partial t}(\vec{r}, t) = \nabla \cdot \left( D_e(T_e, T_l) \nabla T_e(\vec{r}, t) \right) - g \cdot (T_e(\vec{r}, t) - T_l(\vec{r}, t)) + B(\vec{r}, t),$$

(2)

$$\frac{\partial T_l}{\partial t}(\vec{r}, t) = D_l \cdot \Delta T_e(\vec{r}, t) + g \cdot (T_e(\vec{r}, t) - T_l(\vec{r}, t)).$$

(3)

Analyzing the data we find that with reasonable parameters ($D_l = 0.0005 \text{ cm}^2 \text{s}^{-1}$, $D_e = 0.05 \text{ cm}^2 \text{s}^{-1}$) the energy in the electronic system dissipates on a timescale of a few ten femtoseconds (see figure 8), whereas the energy transfer into the phonon system requires picoseconds. That is, the energy density that remains after 30 fs is much too low to induce a temperature close to the melting temperature. To create a high enough energy density in this scenario $g$ would have to be three orders of magnitude larger which is non-physical.

If the energy transfer happens via electron–electron and electron–phonon scattering the diffusion coefficient is directly related to the scattering cross section of two particles. In the case of highly excited electrons the scattering cross section between a hot electron and a cold one is small because they are energetically too different from each other. Only by transferring energy to the phononic system can the energy (and the temperature) of the electrons decrease and thus the diffusivity increase. To take this into account one could use a temperature dependent diffusivity (see e.g. [24]) for the electronic system instead of a constant diffusion. In an earlier work a Boltzmann transport ansatz has been used to calculate the thermal conductivity $K_e(T_e)$ and the heat capacity $C_e(T_e)$ [25]. In principle, $D(T_e, T_l)$ could be calculated from these values but solving the Boltzmann transport equations requires an enormous computational effort. Here, we discuss an approach which treats the excited electrons as an electron gas with a very low-density [26]:

$$D(T) = \frac{2 k_B}{\pi m_e} \frac{T_e}{a T^2_e + b T^2_l},$$

(4)
Figure 8. Energy density on the surface for \( g \approx 1 \times 10^{18} \text{W (m}^3\text{K})^{-1} \) after \( t = 32 \text{ fs} \). The diffusion of the energy within the electronic system is treated with a constant diffusion coefficient (see text).

with \( k_B \) the Boltzmann constant, \( m_e \) the electron mass, \( T_e = \sqrt{2E_e/C_e} \) and \( T_l = 2E_l/(3Nk_b) \). The parameters \( a \) and \( b \) correspond to the electron–electron scattering and the electron–phonon scattering, respectively. For \( b \), to our knowledge neither experimental nor theoretical values exist and \( b \) is therefore treated as a fitting parameter. The parameter \( a = 9 \times 10^9 (\text{K}^2 \text{s})^{-1} \) can be calculated from resistance values measured at low temperatures [27] if electron–phonon scattering is neglected. As \( D(T) \) is proportional to \( 1/T_e \) for \( T_l \ll T_e \) the diffusion is very ineffective at high lattice temperatures (see figure 9). Thus, the excitation within this approach can be confined to a small region, lasting long enough to feed sufficient energy into the much slower phonon system characterized by a constant diffusion coefficient. Solving the diffusion equations within this approach, maxima of phonon energies are compatible with the melting temperature and typically occur on a picosecond timescale, which seems quite reasonable.

That is, within the two-temperature model the timescale problem discussed above could be overcome by the introduction of a temperature-dependent diffusion coefficient. This does not, however, solve the basic problem of the two-temperature model itself that the system is not in thermal equilibrium during the excitation process and thus important physical quantities, such as the temperature are ill-defined. The conversion of energy into electron temperatures, e.g. by using the heat capacity would only be correct if we assume that the thermalization of the electronic excitation happens either very fast or the distribution is fermi-like from the beginning. For metals, it has been shown that the thermalization of a non-thermally excited electron gas requires 10–100 fs [28, 29]. In the case of an insulator, this time should be even longer due to long-lived excitations, such as excitons. In this sense, the temperatures should be interpreted as a quantity to parameterize the energy density but not as a real temperature.

Finally, we would like to discuss the possibility that the creation of nanodots may not at all be the result of a thermal process but is linked to a direct coherent excitation of atoms. This so-called non-thermal melting has been observed for semiconductors like InSb and is due to the efficient excitation of optical phonons by intense laser pulses [30]. A prerequisite for
this process is the excitation of an electron–hole plasma by the intense laser pulse [31]. With ions, field strengths of similar intensity can be achieved and thus a dense enough electron–hole plasma could be created. On the basis of the current data it is not possible to check whether this process exists. In any case it could not be treated within the two-temperature model and is thus beyond the scope of this paper.

5. Conclusions

We have shown that with swift heavy ions chains of individual hillocks can be created on SrTiO$_3$ surfaces if the irradiation takes place under glancing angles. The length of the chains can be easily controlled by varying the glancing angle. While the length of the chains is independent of the azimuthal angle, the hillock separation within the chains is not. This is a clear indication that the exact spatial distribution of the electrons has to be taken into account in order to understand the hillock formation. We have demonstrated how within the two-temperature model the electron–phonon coupling constant can be obtained from the dependence of the chain length on the angle of incidence.

Applying the two-temperature model to our data we find that the electronic excitation dissipates too fast to deliver enough energy to the phonon system. This problem could be overcome by using a temperature-dependent diffusion coefficient, yielding reasonable timescales for the phonon heating in the range of several tens of picoseconds. However, one has to keep in mind that only relatively few electrons with rather high energies are created by the moving ion. Thus, a model based on temperatures and describing a diffusive transport might not be appropriate at all. Instead, the transport would be better described applying a Boltzmann transport formalism which is part of the ongoing research in our group.

Acknowledgments

We thank R Meyer for calculating the electron density and for stimulating discussions. Financial support by the DFG - SFB616: Energy dissipation at surfaces is gratefully acknowledged.

*New Journal of Physics* **10** (2008) 053007 (http://www.njp.org/)
The experiments were performed at the IRRSUD beamline of the Grand Accelerateur National d’Ions Lourds (GANIL), Caen, France.

References

[1] Awazu K, Wang X, Fujimaki M, Komatsubara T, Ikeda T and Ohki Y 2006 Structure of latent tracks in rutile single crystal of titanium dioxide induced by swift heavy ions J. Appl. Phys. 100 044308

[2] Khalfaoui N, Görlich M, Müller C, Schleberger M and Lebius H 2006 Latent tracks in CaF₂ studied with atomic force microscopy in air and in vacuum Nucl. Instrum. Methods B 245 246–9

[3] El-Said A S, Cranney M, Ishikawa N, Iwase A, Neumann R, Schwartz K, Toulemonde M and Trautmann C 2004 Study of heavy-ion induced modifications in BaF₂ and LaF₃ single crystals Nucl. Instrum. Methods B 218 492–7

[4] Müller A, Neumann R, Schwartz K and Trautmann C 1998 Scanning force microscopy of heavy-ion tracks in lithium fluoride Nucl. Instrum. Methods B 146 393–8

[5] Seitz F and Köhler J 1956 Displacement of atoms during irradiation Solid State Phys. 2 305

[6] Toulemonde M, Dufour C and Paumier E 1992 Transient thermal process after a high-energy heavy-ion irradiation of amorphous metals and semiconductors Phys. Rev. B 46 14362

[7] Meftah A, Constantini J M, Khalfaoui N, Boudjadar S, Stoqert J P, Studer F and Toulemonde M 2005 Experimental determination of track cross-section in Gd₃Ga₅O₁₂ and comparison to the inelastic thermal-spike model applied to several materials Nucl. Instrum. Methods B 237 563

[8] Akcöltekin E, Peters Th, Meyer R, Duvenbeck A, Klusmann M, Monnet I, Lebius H and Schleberger M 2007 Creation of multiple nanodots by single ions Nat. Nanotechnol. 2 290–4

[9] Carvalho A M J F, Marinoni M, Touboul A D, Guasch C, Lebius H, Ramonda M, Bonnet J and Saigné F 2007 Discontinuous ion tracks on silicon oxide on silicon surfaces after grazing angle heavy ion irradiation Appl. Phys. Lett. 90 073116

[10] Vorobyova I V 1998 Tracks formation on LiF crystal surface due to grazing incidence of 1 MeV/u Sn ions Nucl. Instrum. Methods B 146 379–84

[11] Klaumünzer S 2006 Thermal-spike models for ion track physics: a critical examination Mat.-Fys. Medd. K. Dan. Vidensk. Selsk. 52 293

[12] Shima K, Kuno N and Yamanouchi M 1989 Systematics of equilibrium charge distributions of ions passing through a carbon foil over the ranges Z = 4–92 and E = 0.002–6 MeV/u Phys. Rev. A 40 3557

[13] Ziegler J F and Biersack J P 2008 The stopping and range of ions in matter (SRIM) http://www.srim.org

[14] Horcas I, Fernández R, Gómez-Rodríguez J M, Colchero J, Gómez-Herrero J and Baro A M 2007 WSxM: a software for scanning probe microscopy and a tool for nanotechnology Rev. Sci. Instrum. 78 013705

[15] Itoh M, Wang R, Inaguma Y, Ymaguchi T, Shan Y-J and Nakamura T 1999 Ferroelectricity induced by oxygen isotope exchange in strontium titanate perovskite Phys. Rev. Lett. 82 3540

[16] The abinit code is a common project of the Université Catholique de Louvain, Corning Incorporated and other contributors. http://www.abinit.org

[17] Fuchs M and Scheffler M 1999 Ab initio pseudopotentials for electronic structure calculations of polyatomic systems using density-functional theory Comput. Phys. Commun. 119 67–98

[18] Perdew J P, Burke K and Ernzerhof M 1996 Generalized gradient approximation made simple Phys. Rev. Lett. 77 3865–8

[19] Osmani O, Duvenbeck A, Akcöltekin E, Meyer R, Lebius H and Schleberger M 2008 Ab initio calculation of electronic stopping power along glancing swift heavy ion tracks in perovskites J. Phys.: Condens. Matter submitted (Preprint 0801.3381v1) [cond-mat.mtrl-sci]

[20] Lindhard J and Scharff M 1961 Energy dissipation by ions in the keV region Phys. Rev. 124 128
[21] de Lingy D and Richet P 1996 High-temperature heat capacity and thermal expansion of SrTiO$_3$ and SrZrO$_3$ perovskites Phys. Rev. B 53 3013
[22] Groeneveld R H M, Sprik R and Lagendijk A 1995 Femtosecond spectroscopy of electron–electron and electron–phonon energy relaxation in Ag and Au Phys. Rev. B 51 11433
[23] Caron M, Rothard H, Toulemonde M, Gervais B and Beune M 2006 Theoretical and experimental study of electron temperatures in heavy ion tracks from Auger electron spectra and thermal spike calculations Nucl. Instrum. Methods B 245 36
[24] Duvenbeck A and Wucher A 2005 Low-energy electronic excitation in atomic collision cascades: a nonlinear transport model Phys. Rev. B 72 165408
[25] Schiwiynet G, Xiao G, Luderer E and Grande P L 2000 Auger electrons from ion tracks Nucl. Instrum. Methods B 164–5 353
[26] Baranov I A, Martynenko Yu V, Tsepelevich S O and Yavlinskii Yu N 1988 Inelastic sputtering of solids by ions Sov. Phys.—Usp. 31 1015
[27] Okuda T, Nakinishi K, Miyasaka S and Tokura Y 2001 Large thermoelectric response of metallic perovskites Sr$_{1-x}$La$_x$TiO$_3$(0 ≤ x ≤ 0.1) Phys. Rev. B 63 113104
[28] Schmuttenmaer C A, Aeschlimann M, Elsayed-Ali H E, Miller R J D, Mantell D A, Cao J and Gao Y 1994 Time-resolved two-photon photoemission from Cu(100): energy dependence of electron relaxation Phys. Rev. B 50 8957
[29] Rethfeld B, Kaiser A, Vicanek M and Simon G 2002 Ultrafast dynamics of nonequilibrium electrons in metals under femtosecond laser irradiation Phys. Rev. B 65 214303
[30] Rousset A, Rischel C, Fourmaux S, Uschmann I, Sebban S, Grillon G, Balcou Ph, Förster E, Geindre J P, Audebert P, Gauthier J C and Hulin D 2001 Non-thermal melting in semiconductors measured at femtosecond resolution Nature 410 65
[31] Stampfl P and Bennemann K H 1990 Theory for the instability of the diamond structure of Si, Ge, and C induced by a dense electron–hole plasma Phys. Rev. B 42 7163