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Particle reflection coefficients during beryllium and tungsten bombardment by various atoms

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Using computer simulation, the particle reflection coefficients for Be and W targets were calculated in the 10 eV−100 keV energy range of incident atoms. H, D, T, He, Be, C, N, O, Ne, Ar, W were chosen as bombarding particles. The influence on reflection coefficients of the electronic stopping model, the surface potential barrier and the structure of the target (crystal, amorphous body) is shown.

Keywords: reflection coefficients, atomic particles, beryllium, tungsten, ITER tokamak.

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Introduction

Deuterium-tritium plasma is to be used in the ITER tokamak. As known, tungsten has been chosen as a divertor material for ITER tokamak. Beryllium is a promising material for the first wall. Accordingly, this study investigates the beryllium and tungsten particle reflection. Atom reflection from structural materials affects the energy and material balance of plasma. Particle reflection shall be also considered for ion implantation, since it affects the number of implanted atoms.

The experimental data on reflection coefficients for Be and W is extremely limited [1,2].

Unfortunately, we do not know the theoretical formula describing the dependence of reflection coefficients on the energy of bombarding particles. A chapter in [3] is devoted to discussion of possible theoretical approaches to the description of particle scattering on the surface. To describe light atom scattering in heavy targets, a set of empirical formulas is offered in [4–7]. An attempt is made in [8] to describe reflection coefficients in terms of relation of path length to transport cross-section. A similar attempt has been made recently in [9].

Computer simulation is widely used to study atomic particle scattering on materials surface [3,10]. Commonly used SRIM code [11] is based on the binary collision approximation (hereinafter referred to as BCA) that was proposed in [12]. Among other publications, it is important to note reflection coefficient calculations using molecular dynamics methods [13,14] and [15] where the surface shape effect on reflection coefficients was investigated. Our study [16] used multiple scattering of hydrogen atoms on the metal surface to obtain the information on the atom-surface interaction potential.

The presence of potential well results in particle attraction at long internuclear distances and affects reflection coefficients. Our studies [17–20] calculated the reflection coefficients of hydrogen and helium isotopes in the energy range from 100 eV to 10 keV. Helium atoms are the nuclear fusion reaction products, therefore scattering coefficients of helium atoms at the same targets were calculated. The energy range of bombarding particles was expanded herein to 10 eV−100 keV. The calculations used the potentials calculated in the density functional theory (DFT) approach with spectroscopic data correction of the potential well parameters [21]. The objective of the study included the calculation of reflection coefficients for hydrogen isotopes and data acquisition for He atoms and various impurity atoms admission of which may be used for cooling edge plasma.

1. Calculation procedure

Calculations were performed using a code developed by us in [22], that is based on the Monte Carlo method. To collect the required statistical data, 1 000 000 bombarding particle trajectories were usually calculated with randomly selected initial conditions with equally probable distribution on the target surface. The bombarding particle trajectory in solid body is considered in binary collision approximation (BCA). In this approximation, atomic particle scattering is considered as a sequence of binary collisions with solid body atoms. For this, the particle trajectory is replaced with trajectory asymptotes. BCA acceptance criteria are addressed in [10]. The presence of short-range order in polycrystalline target scattering simulation is considered as follows. An atom cluster randomly oriented in space is set. The distance between atoms is determined from the target density. When the next collision occurs, the cluster orientation in space is simulated again. The surface is defined as a random cut of the initial cluster. Thermal

vibrations of the target atoms are taken into account. The calculations were carried out at room temperature.

Recoil particle trajectories were calculated using many-particle potentials determined using the density functional theory [23–27] with potential well parameters correction [28]. The correction was carried out considering the experimental data on the well depth and potential energy minimum position obtained from the spectroscopic measurements [29–32].

To describe the electronic stopping, we used reliable experimental data for aluminum [33] and scaling up to the difference in electron densities of beryllium or tungsten target material using the procedure proposed in [34]. A correction for multiple collisions was introduced into the data [35]. The energy loss was calculated as a product of trajectory length between consecutive collisions and „electronic stopping per unit length of the trajectory".

The difference of our calculations form previous calculations is as follows: more accurate interaction potentials are used, for large-angle scattering, the scattering angle is calculated accurately without using approximated („magic") formulas used in SRIM. The effect of surface potential barrier is considered. The correction for multiple collisions is introduced in the electronic stopping data [35].

2. Reflection coefficients simulation results

Figure 1 shows reflection coefficients of H, D, T, He, Be, C, N, O, Ne in beryllium target scattering at bombarding particle energies 10 eV–100 keV. Attention is focused on data grouping for systems with $M_1 < M_2$ and $M_1 > M_2$, where M_1 is the bombarding particle atomic mass, M_2 is the target atomic mass. This is not surprising, because for $M_1 > M_2$, single scattering at angles larger that 90° does not occur and only multiple scattering contributes to reflection coefficients. Reflection coefficients reduction also takes place with increase of M_1.

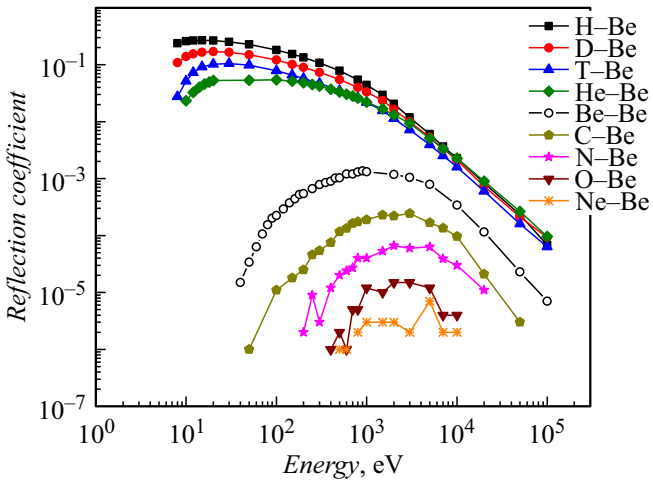

Figure 1. Calculated particle reflection coefficients or beryllium target depending on the energy for bombarding H, D, T, He, Be, C, N, O, Ne atoms. For Be–Be system, the planar potential barrier calculation is provided.

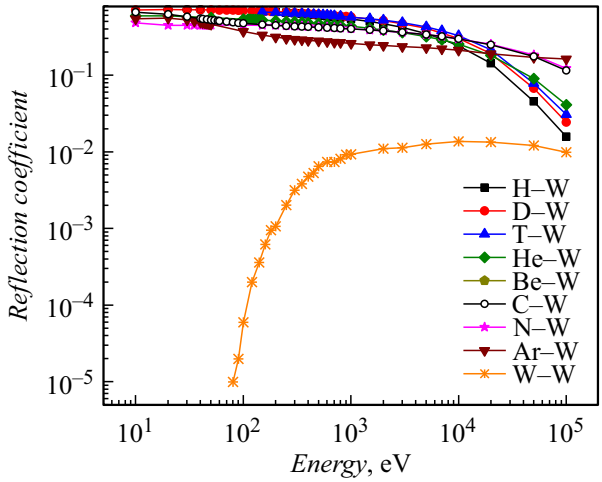

Figure 2. Calculated particle reflection coefficients for tungsten target depending on the energy for bombarding H, D, T, He, Be, C, N, Ar, W atoms. Data for W–W system is provided for the planar potential barrier.

Figure 2 shows reflection coefficients of H, D, T, He, Be, C, N, Ar, W atoms from the tungsten surface. In this case, $M_1 < M_2$ is not met only for W–W collisions. As shown in Figure 2, the reflection coefficient for W–W falls rapidly due to the exclusion of single scattering at angles larger than 90°.

Calculation for collision of similar particles shall be clarified. Computer modeling allows marking of a bombarding particle and tracking its escape from the surface. It is impossible to distinguish a sputtered particle from a reflected particle in the experiment. For symmetric systems ($M_1 = M_2$), single collision does not result in particle escape from the target. Energy spectrum of reflected particles is characterized by a large number of low-energy particles. For W–W system, there is a potential well that results in the occurrence of the potential barrier near the surface. When the potential barrier is present, bombarding particle acceleration by the potential barrier during entrance into a solid body and the presence of the potential barrier during particle escape shall be considered. In case of spherical barrier for the surface consisting of spikes, the bombarding particle energy E_0 shall be higher that the sublimation energy E_s. In case of the planar barrier, the condition $E_0 \cdot \cos^2\theta > E_s$ shall be met for a smooth surface, where θ is the particle escape angle with respect to normal to surface. As shown in Figure 3, the presence of surface barriers significantly changes the reflection coefficients at low energies and causes the occurrence of thresholds. Sputtering coefficients are approximately 100 times higher than reflection coefficients. Thresholds for these two processes almost coincide (during curve normalization). The obtained

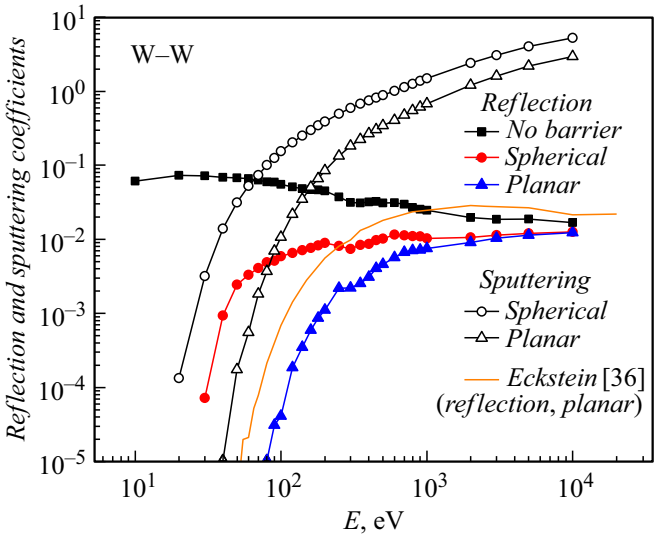

Figure 3. W–W system. Comparison of reflection and sputtering coefficients for spherical and planar surface barriers and for the case without a barrier (reflectance). The line shows the reflection coefficient calculation from [36] for the planar barrier case.

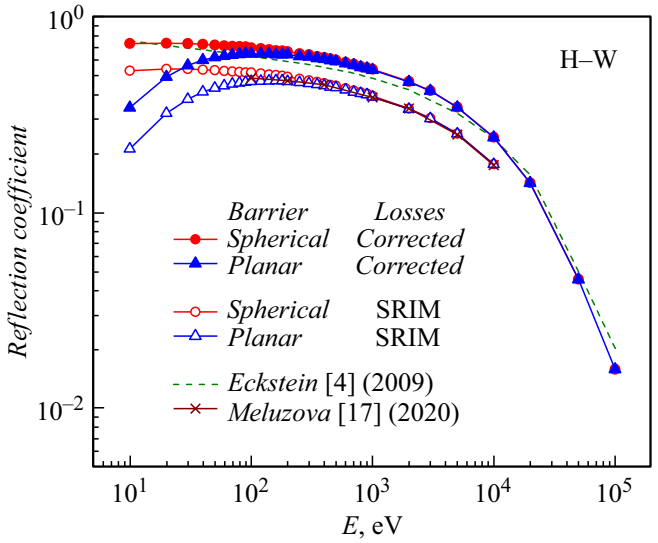

Figure 4. Reflection coefficients for H–W system. Calculation for two electronic stopping models is provided: SRIM package and dependence corrected for multiple collisions [35], for spherical and planar barriers. For comparison, Eckstein's [4] and Meluzova's [17] calculations are provided.

data for reflection in case of the planar surface barrier are in satisfactory agreement with Eckstein's calculation data [36].

For H–W collisions, there is also a potential well 4.6 eV in depth, and particle acceleration during target entrance and deceleration during escape were carried out by sublimation energy replacement with the potential well depth.

As shown in Figure 4, consideration of the presence of surface barriers significantly changes the course of curves at low collision energies. Eckstein's calculation coincides with out calculation for the case when there is no any surface barrier and when a modified inelastic energy loss model is used. Data from [17] is lower by 30%. This appeared to be due to the use of various electronic stopping models. We have repeated the calculation using the data from SRIM database, and the calculation coincided with Meluzova's data from [17]. We have shown in [35] that SRIM database contains data for electronic stopping per unit length of the projective trajectory. At collision energies lower than 10 keV, this data must be corrected for trajectory distortion due to multiple collisions. Electronic stopping data for these models are shown in Figure 5.

Modified data for energy lower than 17 keV are well described by $dE/dx = 1.488 \cdot E^{0.722}$, whereby dE/dx are expressed in eV/Å, and E are expressed in keV. As shown in Figure 4, the change of electronic stopping significantly affects the particle reflection coefficients.

As shown in Figure 6, *a*, our calculation for D–W system is above the experimental data and almost coincides with the calculations in SDTrimSP, MARLOWE and PTr (for a smooth surface). Our data also agree quite well with PARCAS calculations (molecular dynamics calculation). Figure 6, *b* shows that our calculation for He–W system is between Eckstein's and Amano's experimental data and lower than SDTrimSP, ACAT, MARLOWE (amorphous target) and PTr (for smooth surface) calculations. TAVERN calculation is lower than our data. For Ar–W system, our calculation is lower than the data obtained using SDTrimSP, ACAT and MARLOWE.

Figure 7 shows that data for crystalline and amorphous targets are different. For the crystalline target, due to the channeling effect, the bombarding particles enter deeper into the target, and their escape from the target is hindered and causes rapid drop of reflection coefficient. For the

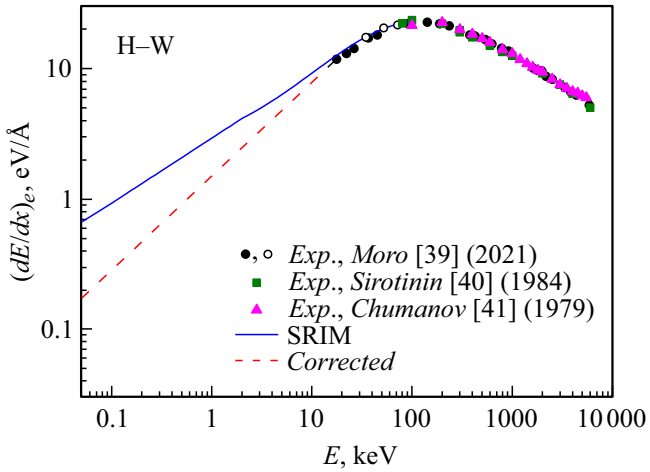

Figure 5. Dependence of electronic stopping on collision energy for H–W system. Dots — experimental data from [38-40]. Solid line — SRIM package data. Dashed line — modified data.

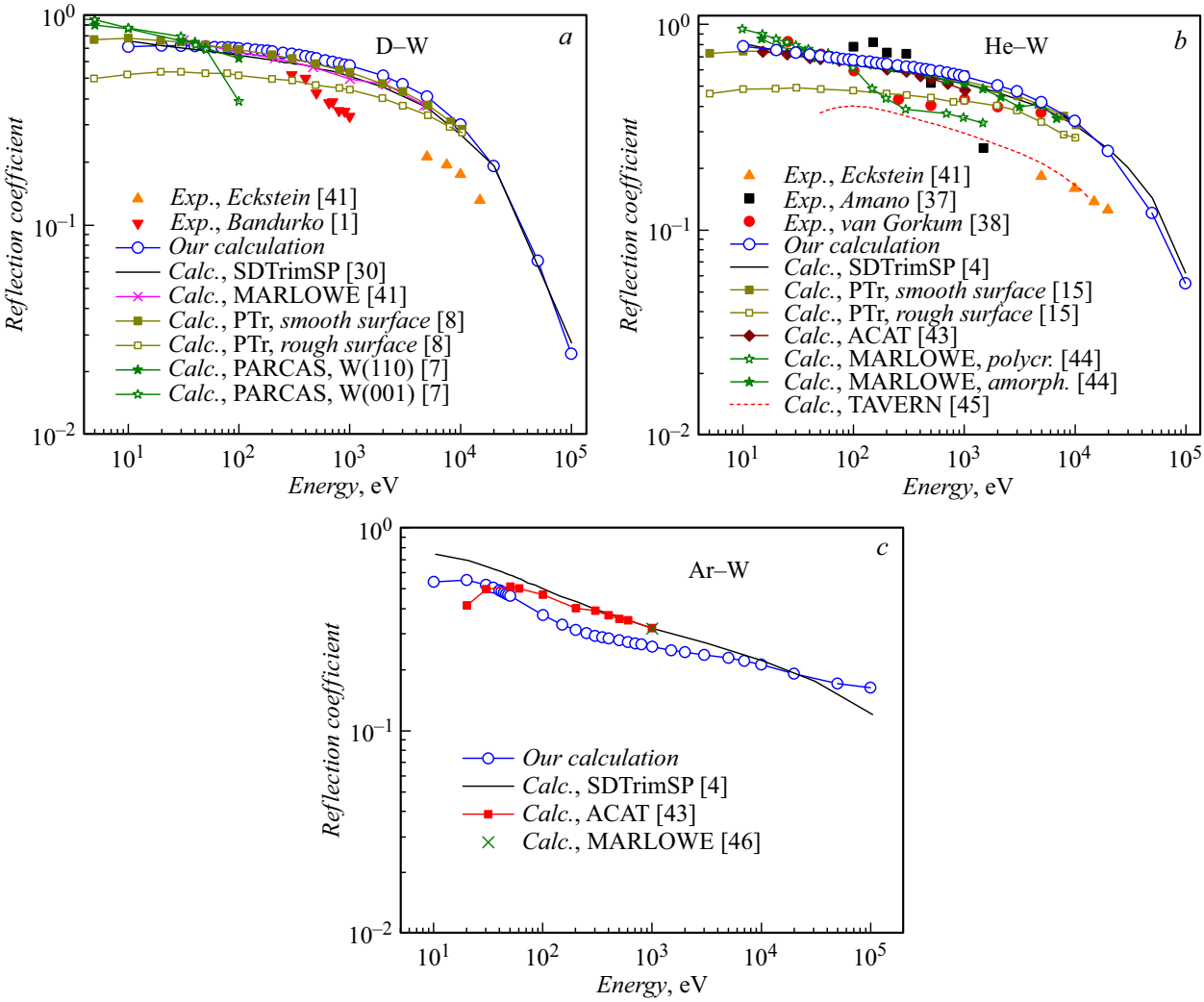

Figure 6. Reflection coefficients for D–W (*a*), He–W (*b*) and Ar–W (*c*) systems.

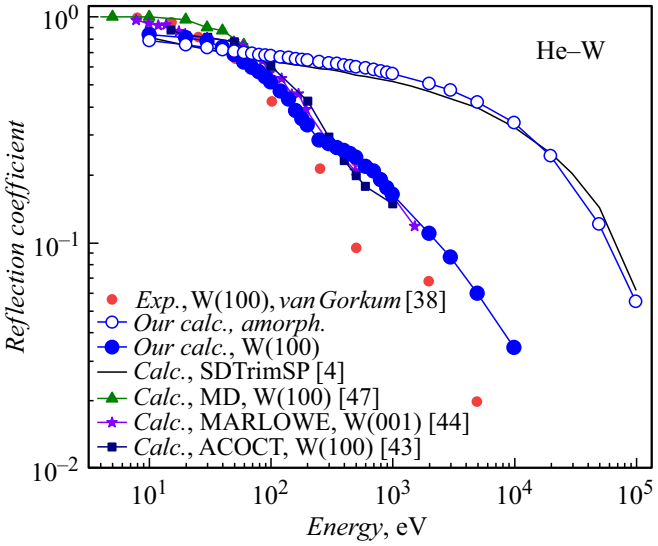

Figure 7. He–W system. Reflection coefficients for crystalline and amorphous target. ACOCT is an ACAT version for crystalline targets.

crystalline target, there is a satisfactory agreement with the experiment [38]. Calculations performed in different software coincide.

Conclusion

Reflection coefficients are calculated for Be and W target bombarding by H, D, T, He, Be, C, N, O, Ne, Ar, W atoms in a wide bombarding atom energy range 10 eV–100 keV. For $M_2 > M_1$, reflection coefficients fall rapidly due to the absence of single scattering contribution. It is shown that consideration of a potential barrier has a major influence on particle reflection coefficients. This has a particular high effect when $M_2 > M_1$. At particle energies of 0.5–1 keV, the difference becomes less apparent.

Consideration of current understanding of the electronic stopping also has a considerable effect on simulation. The example of H–W system shows that correction of electronic stopping for multiple collisions results in the change of the

reflection coefficient by a factor of 1.35 throughout the energy range of interest.

It is commonly known that the calculations are also considerably affected by the target structure (crystal, amorphous body). This difference is demonstrated by He−W system.

In case when there is experimental data, the provided calculations agree well with the experiment and other calculations. The difference of the provided calculations from previous calculations is as follows: more accurate interaction potentials are used, for large-angle scattering, the scattering angle is calculated accurately without using approximated („magic") formulas. The effect of surface potential barrier is considered. The correction for multiple collisions is introduced in the electronic stopping data.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] V.V. Bandurko, N.N. Koborov, V.A. Kurnaev, V.M. Sotnikov, O.V. Zabeyda. J. Nucl. Mater., **176−177**, 630 (1990). DOI: 10.1016/0022-3115(90)90118-7

[2] R.D. Kolasinski, N.C. Bartelt, J.A. Whaley, T.E. Felter, W.R. Wampler. *Fundamental hydrogen Interactions with Beryllium: a Magnetic Fusion Perspective.* SNL Report № SAND2012-2323 (Sandia National Laboratories, Albuquerque, 2012)

[3] V.A. Kurnaev, E.S. Mashkova, V.A. Molchanov. *Otrazhenie legkikh ionov ot poverkhnosti tverdogo tela* (Energoatomizdat, M., 1985) (in Russian)

[4] W. Eckstein. *Reflection (Backscattering).* IPP-17-12 (IPP, Garching, 2009)

[5] R.A. Langley, J. Bohdansky, W. Eckstein, P. Mioduszewski, J. Roth, E. Taglauer, E.W. Thomas, H. Verbeek, K.L. Wilson. Nucl. Fusion, **24**, S9 (1984). DOI: 10.1088/0029-5515/24/S1/001

[6] T. Tabata, R. Ito, Y. Itikawa, N. Itoh, K. Morita. Atomic Data and Nucl. Data Tables, **28** (3), 493 (1983). DOI: 10.1016/0092-640X(83)90004-9

[7] E.W. Thomas, R.K. Janev, J. Smith. J. Nucl. Mater., **69** (4), 427 (1992). DOI: 10.1016!0168-583X(92)95298-6

[8] R.D. Simovic, J. Vukanic. Radiat. Phys. Chem., **80**, 310 (2011). DOI: 10.1016/j.radphyschem.2010.11.003

[9] V.P. Afanas'ev, L.G. Lobanova, V.I. Shulga. J. Surf. Investig., **17** (1), 78 (2023). DOI: 10.1134/S1027451023010032

[10] W. Eckstein. *Computer Simulation of Ion-Solid Interactions* (Springer, Berlin 1991)

[11] J.F. Ziegler, J.P. Biersack. SRIM — http://www.srim.org

[12] M.T. Robinson, I.M. Torrens. Phys. Rev. B, **9** (12), 5008 (1974). DOI: 10.1103/PhysRevB.9.5008

[13] A. Lasa, C. Björkas, K. Vörtler, K. Nordlund. J. Nucl. Mater., **429** (1−3), 284 (2012). DOI: 10.1016/j.jnucmat.2012.06.012

[14] P.N. Maya. J. Nucl. Mater., **480**, 411 (2016). DOI: 10.1016/j.jnucmat.2016.08.007

[15] D.K. Kogut, N.N. Trifonov, V.A. Kurnaev. Bull. Russ. Academy Sci.: Phys., **72** (7), 969 (2008). DOI: 10.3103/S1062873808070241

[16] P.Yu. Babenko, A.N. Zinoviev, V.S. Mikhailov, D.S. Tensin, A.P. Shergin. Tech. Phys. Lett., **48** (7), 50 (2022). DOI: 10.21883/TPL.2022.07.54039.19231

[17] D.S. Meluzova, P.Yu. Babenko, A.P. Shergin, A.N. Zinoviev. J. Surf. Investig., **14**, 738 (2020). DOI: 10.1134/S102745102004014X

[18] P.Yu. Babenko, A.N. Zinoviev, A.P. Shergin. J. Surf. Investig., **13**, 712 (2019). DOI: 10.1134/S1027451019040207

[19] D.S. Meluzova, P.Yu. Babenko, A.P. Shergin, K. Nordlund, A.N. Zinoviev. NIMB, **460**, 4 (2019). DOI: 10.1016/j.nimb.2019.03.037

[20] P.Yu. Babenko, A.M. Deviatkov, D.S. Meluzova, A.P. Shergin, A.N. Zinoviev. NIMB, **406**, 538 (2017). DOI: 10.1016/j.nimb.2016.12.043

[21] A.N. Zinoviev, P.Yu. Babenko, K. Nordlund. NIMB, **508**, 10 (2021). DOI: 10.1016/j.nimb.2021.10.001

[22] D.S. Meluzova, P.Yu. Babenko, A.P. Shergin, A.N. Zinoviev. J. Surf. Investig., **13**, 335 (2019). DOI: 10.1134/S1027451019020332

[23] F. Granberg, J. Byggmästar, K. Nordlund. J. Nucl. Mater., **556**, 153158 (2021). DOI: 10.1016/j.jnucmat.2021.153158

[24] C. Bjorkas, K. Nordlund. J. Nucl. Mater., **439**, 174 (2013). DOI: 10.1016/j.jnucmat.2013.04.036

[25] A. Lyashenko, E. Safi, J. Polvi, F. Djurabekova, K. Nordlund. J. Nucl. Mater., **542**, 152465 (2020). DOI: 10.1016/j.jnucmat.2020.152465

[26] C. Bjorkas, N. Juslin, H. Timko, K. Vortler, K. Nordlund, K. Henriksson, P. Erhart. J. Phys.: Condens. Matter, **21**, 445002 (2009). DOI: 10.1088/0953-8984/21/44/445002

[27] M.V. Prokofyev, V.V. Svetukhin, M.Yu. Tikhonchev. Izv. Samarskogo NTs RAN, **15** (4), 1024 (2013) (in Russian).

[28] A.N. Zinoviev, P.Yu. Babenko, K. Nordlund. NIMB, **508**, 10 (2021). DOI: 10.1016/j.nimb.2021.10.001

[29] Y.R. Luo. *Comprehensive Handbook of Chemical Bond Energies* (CRC Press, Boca Raton, 2007)

[30] B. Darwent. *Bond Dissociation Energies in Simple Molecules* (U.S. National Bureau of Standards, 1970)

[31] A.A. Radzig, B.M. Smirnov. *Reference Data on Atoms, Molecules, and Ions* (Springer, Berlin, 1985) DOI: 10.1007/978-3-642-82048-9

[32] B.P. Nikol'sky, *Spravochnik khimika* (Khimiya, L., 1966) (in Russian).

[33] D. Primetzhofer, S. Rund, D. Roth, D. Goebl, P. Bauer. Phys. Rev. Lett., **107** (16), 163201 (2011). DOI: 10.1103/PhysRevLett.107.163201

[34] A. Mann, W. Brandt. Phys. Rev. B, **24** (9), 4999 (1981). DOI: 10.1103/PhysRevB.24.4999

[35] A.N. Zinoviev, P.Yu. Babenko. JETP Lett., **115** (9), 560 (2022). DOI: 10.1134/S0021364022100526

[36] W. Eckstein. *Calculated Sputtering, Reflection and Range Values* (IPP, Garching, 2002)

[37] J. Amano, D.N. Seidman. J. Appl. Phys., **52** (11), 6934 (1981). DOI: 10.1063/1.328647

[38] A.A. van Gorkum, E.V. Kornelsen. Rad. Eff., **52** (1−2), 25 (1980). DOI: 10.1080/00337578008210013

[39] M.V. Moro, P.M. Wolf, B. Bruckner, F. Munnik, R. Heller, P. Bauer, D. Primetzhofer. NIMB, **498**, 1 (2021). DOI: 10.1016/j.nimb.2021.04.010

[40] E.I. Sirotinin, A.F. Tulinov, V.A. Khodyrev, V.N. Mizgulin. NIMB, **4**, 337 (1984). DOI: 10.1016/0168-583x(84)90577-9

[41] V.Y. Chumanov, S.Z. Izmailov, G.P. Pokhil, E.I. Sirotonin, A.F. Tulinov. Phys. Status Solidi A, *53*, 51 (1979). DOI: 10.1002/pssa.2210530104
[42] W. Eckstein, H. Verbeek. *Data on Light Ion Reflection* (IPP, Garching, 1979)
[43] Y. Yamamura. NIMB, **33** (1–4), 429 (1988). DOI: 10.1016/0168-583X(88)90599-X
[44] M.T. Robinson. J. Nucl. Mater., **103**, 525 (1981). DOI: 10.1016/0022-3115(82)90652-3
[45] D.P. Jackson, W. Eckstein. Nucl. Instr. Meth., **194** (1–3), 671 (1982). DOI: 10.1016/0029-554X(82)90602-4
[46] O.S. Oen, M.T. Robinson. AIP Conf. Proc., **111** (1), 171 (1984). DOI: 10.1063/1.34417
[47] V. Borovikov, A.F. Voter, X.-Z. Tang. J. Nucl. Mater., **447** (1–3), 254 (2014). DOI: 10.1016/j.jnucmat.2014.01.021

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