Molecular dynamics simulations of nitrogen ion channeling in α-titanium target

M. Lebeda[1, 2, 3], J. Drahokoupil[3], P. Vlčák[1]
[1]*Department of Physics, Faculty of Mechanical Engineering, Czech Technical University in Prague*
[2]*Department of Solid State Engineering, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague*
[3]*Department of Material Analysis, Institute of Physics, Czech Academy of Sciences*

INTRODUCTION

Ion implantation and channeling effect in α-Ti

Implanting N ions into Ti-based materials improves their properties such as hardness, corrosion resistance, or friction coefficient. During the implantation, significant number of ions can be guided through crystal channels, resulting into larger penetration depths (i.e., ion channeling) and smaller number of crystal defects. An important characteristic of ion-implanted materials is ion distribution across the depth of the target. Depending on the parameters of implantation, depth distributions can be strongly affected by the channeling effect. In this work, we used molecular dynamics (**MD**) simulations to predict the N ion channeling in hex. α-Ti at 0.5-4 keV kinetic energies, different surface orientations, target temperature, and incident angle.

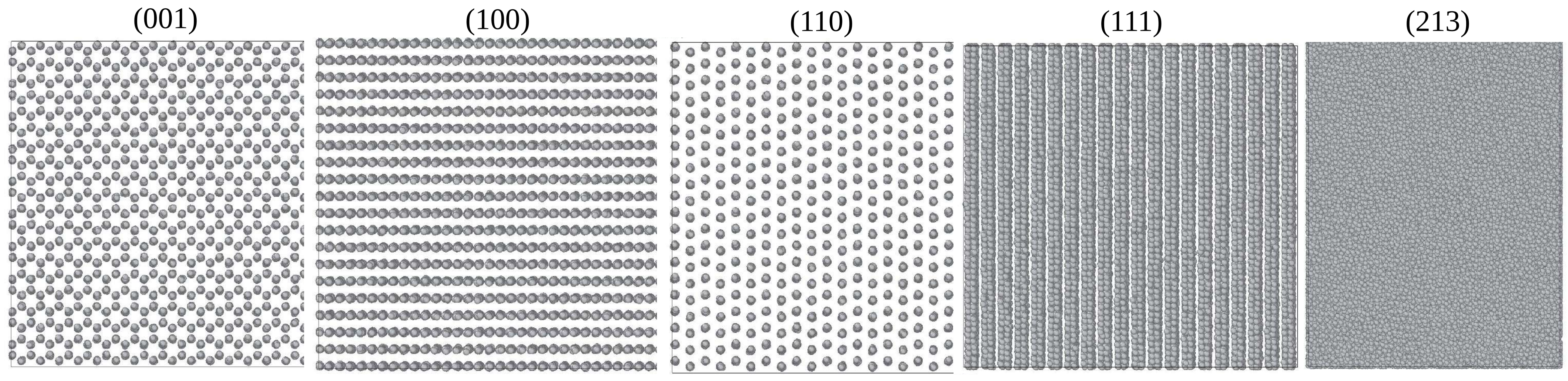


Fig. 1: Surface orientations of α-Ti used for MD simulations of N ion implantation. Different channeling effect is expected for the first four leftmost crystallographic planes. Ti atomic radii were reduced to clearly illustrate crystal channels.

RESULTS

Depth distributions and ion channeling for different kinetic energies, target temperature and incident angles

Fig. 2: MD predictions of **implanted nitrogen depth distributions in α-Ti** at 0.5 keV **(a)**, 2 keV **(b)** and 4 keV **(c)** initial ion energies, 300 K target temperature, and perpendicular ion incidence into four expected channeling crystal surface orientations and one non-channeling orientation. Percentages of channeling ions as compared to nonchanneling orientation are estimated in **(d)**.

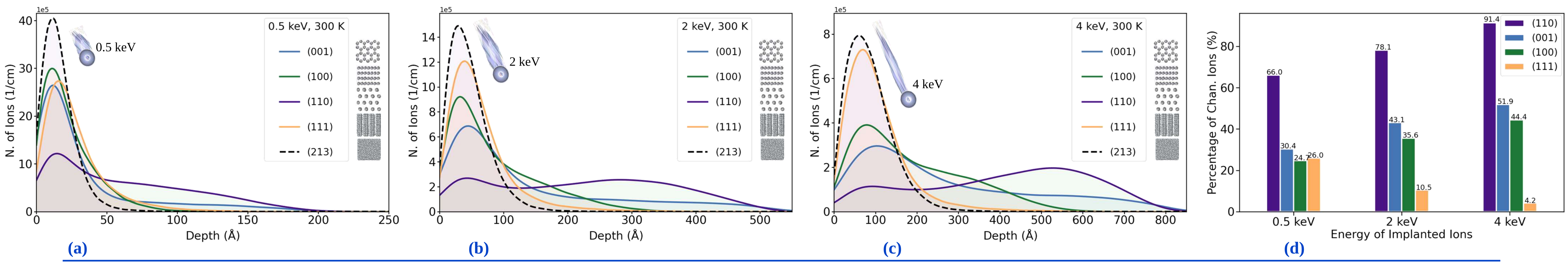


Fig. 3: MD predictions of **target temperature effect** on implanted nitrogen depth distributions in α-Ti at 2 keV initial ion energy and perpendicular incidence into (110) **(a)**, (001) **(b)**, and (100) **(c)** channeling target surface orientations. Changes of percentages of channeling ions with target temperature as compared to nonchanneling orientation are estimated in **(d)**.

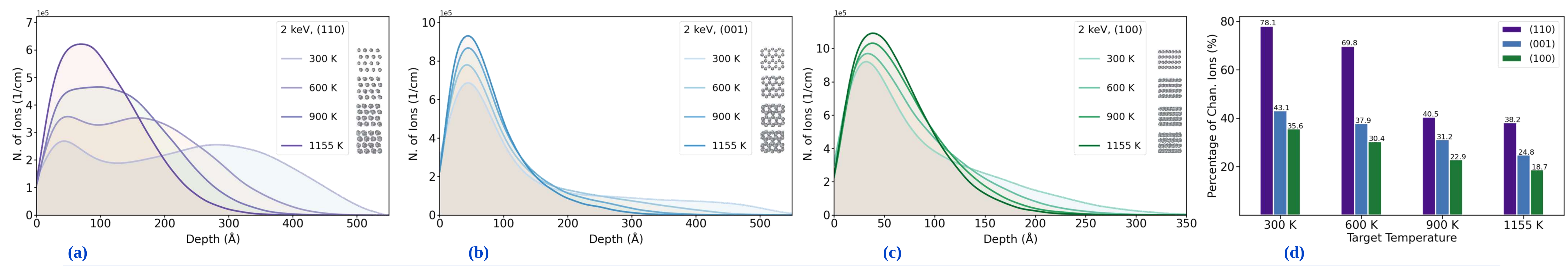
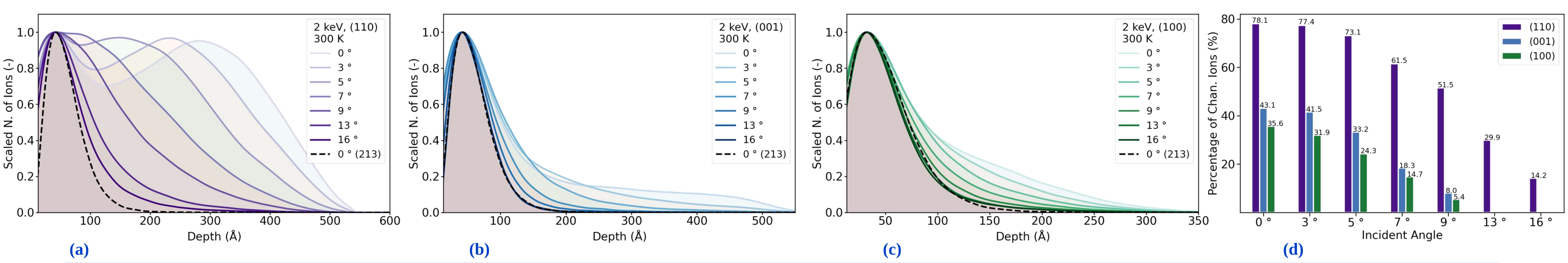


Fig. 4: MD predictions of **incident angle effect** on implanted nitrogen depth distributions in α-Ti at 2 keV initial ion energy and (110) **(a)**, (001) **(b)**, and (100) **(c)** channeling target surface orientations. Changes of percentages of channeling ions with incident angle as compared to nonchanneling orientation are estimated in **(d)**.



CONCLUSIONS

- Using molecular dynamics (MD) simulations, we predicted nitrogen depth distributions in α-Ti target, resulting from the ion implantation at 0.5-4 keV kinetic energies into four expected channeling α-Ti crystal surface orientations and one nonchanneling orientation.
- The most dominant channeling effect was observed for a perpendicular incident into (110) plane, under which a new local maximum started to appear in higher depth with increasing ion energies. At 4 keV, this maximum became a global maximum. For other channeling planes except the (111), percentages of channeling ions were increasing with increasing kinetic energies.
- Effects of target temperature and ion incident angle on MD simulated nitrogen depth distributions were explored and quantified. In accordance with the expectations, increasing target temperature led to a significant but not complete suppression of channeling.

METHODS

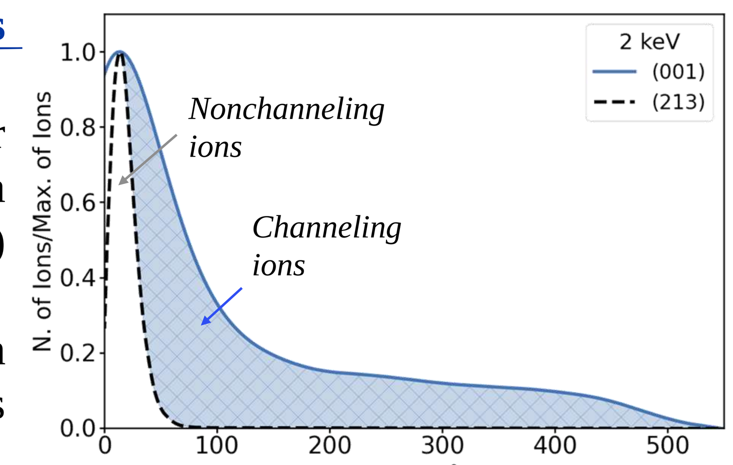
Molecular dynamics, channeling quantification and depth distributions

Molecular dynamics simulations

#LAMMPS
#efficient algorithm for ion implantation [1]
#2NN-MEAM + ZBL [2] potentials
#electronic stopping power
#adaptive timestep
#velocity Verlet algorithm
#periodic boundaries (*x*, *y*), fixed boundary (*z*)
#α-Ti models from Atomsk

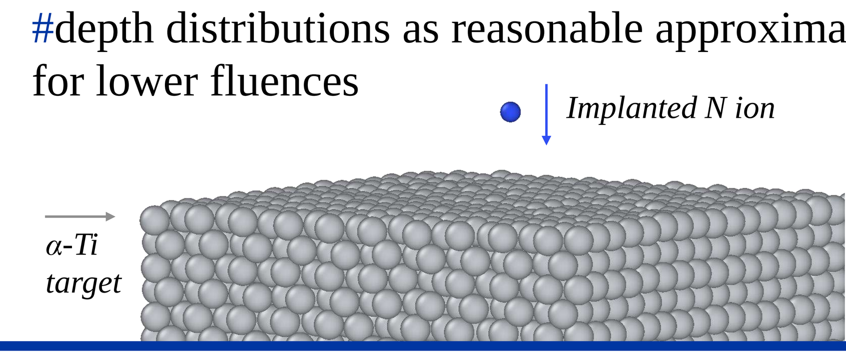
Quantification of channeling ions

#scaled ion depth distributions
#positions of ion maxima for channeling distributions set at a position of nonchanneling (213) distribution
#number of ions in higher depth than in (213) considered as channeling part



Ion depth distributions

#ion depth statistics from over 100 000 ions
#each ion implanted into initial state of α-Ti
#depth distributions as reasonable approximations for lower fluences



References:
[1] Lebeda, M et al., MD simulation of nitrogen ion into α-titanium target. In preparation.
[2] Kim, Y. M. and Lee, B. J. (2008), Acta Materialia, 56(14), pp. 3481–3489.

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