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EVOLUTION OF CRYSTAL MORPHOLOGY UNDER FLOW OF LOW-ENERGY PARTICLES: VACANCY MECHANISM

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Abstract. Initial stages of a crystal surface morphology evolution under local impact of low-energy (of the order of eV and even less) particle beam were studied and a simulation of this process was performed using molecular dynamics. It is shown that change in the crystal morphology can be caused by a vacancy flow towards the spot of the beam incidence along crystallographic directions corresponding to phonon propagation. The mathematical model of this process is proposed and surface profile change rate is estimated. A mechanism of surface roughness development on initially flat surface under impact of uniform particle flux over the whole area is discussed, and morphological stability criterion is found. It is shown that in certain cases one can smooth the surface of the crystal overcoming other mechanisms of spontaneous roughness development.

1. Introduction

Nowadays a lot of attention is paid to study of destruction and change in morphology of crystals [1, 2] under impact of different external factors: mechanical load [3, 4], heating, and laser irradiation [5]. Also mechanisms of destruction of crystals treated by ionic beams and beams of other particles are of interest. Generally, in these studies the change in morphology is caused by one of the following processes: thermal destruction due to local heating of both the sample and absorbing inclusions in its volume; avalanche ionization [6]; various thermochemical processes; mechanochemical phenomena; formation and accumulation of different lattice defects and their subsequent migration. Detailed discussion of these and other mechanisms is presented in reviews [7, 8, 9]. Usually in studies on a particle beam impact high-energy particles in the range of 0.1 - 100 keV [7] are considered, which is much higher than the binding energy of atoms in a crystal (a few eV). Selection of this range is determined by the fact that collisions of such particles with the crystal surface heat it effectively, knock out atoms from the surface [10], and lead to formation of various defects in the volume. The method of molecular dynamics (MD) is frequently used for consideration of these processes [11]. MD within atomistic approach allows one to describe the interaction of the incident particles with the surface and calculate local values of various parameters: temperature and average displacement of atoms from equilibrium position. One of the advantages of this method is that it allows observing such phenomena as generation and movement of defects, for example, formation of craters on the surface and pores in the crystal volume, movement of interstitial atoms, vacancies and many

What happens when the mechanical stresses are negative, i.e. are compressed? From the expression (12) it follows that surface is always stable, and any small perturbation will decay. If we consider other mechanisms of instability development, it is easy to see that usually the amplitude of perturbation growth rate is proportional to the frequency raised to the first or higher powers [30, 32, 34], and is determined by the internal parameters of the system (coefficients of diffusion at a given temperature, equilibrium concentrations, etc.). According to the above proposed mechanism, the rate of growth depends on the frequency linearly. Therefore, via controlling the beam parameters, one can make a "force" that appears under the influence of the beam of particles and leads to decay of perturbation. Such a "force" can suspend growth of perturbations via other mechanisms, and thereby make the surface flat and stable even with respect to long-wave perturbations.

We should note that in the above proposed models, there is no principle difference, what exactly the source of the lattice vibrations arising at the surface is. It may be any low-energy particles: atoms, clusters, molecules of gas, etc. Although in the simulation via MD we considered a beam of neutral particles and purely mechanical interactions, we can assume that the phenomenon of drift of vacancies towards the surface may be observed in the case of any other particles with low energy capable anyhow to transmit momentum to the lattice, for example, photons.

5. Conclusions

We proposed a mechanism of change in morphology of the surface of crystalline solids under the influence of the local beam of low-energy particles, as well as under uniform illumination of the crystal surface. It has been shown that such change may be due to scattering of the lattice vibrations generated near the surface on the vacancies. This causes a drift of vacancies to the spot of the beam incidence. Two modes are showcased: ballistic and diffusion. Their differences are shown and time dependence of the rate of change of the surface profile is found. It is shown that the phonon mean free path l and some other characteristics of the process, for example, the values of Q and p, can be found from the analysis of this dependence. The discovered mechanism of morphology change is most effective when tensile stresses increasing the concentration of vacancies are applied to the crystal. The process of the roughness development on the surface of the elastically-strained crystal was investigated and it is shown that an arbitrary small perturbation of the surface may grow indefinitely under certain conditions because of the nonuniform flow of vacancies towards the surface. Instability appears at spatial frequencies below the critical ω_{cr}, which is determined by intensity of phonon generation, concentration of vacancies, the magnitude and sign of mechanical stress, as well as other parameters of the system. It is shown that if the stresses are negative (compressive), vacancy drift reduces the roughness. This phenomenon can be used to suppress development of instability via other mechanisms even with respect to low-frequency perturbations.

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References

[1] J.A. Hauch, D. Holland, M.P. Marder, H. L. Swinney // *Physical Review Letters* **82** (1999) 3823.
[2] A. Masolin, P.O. Bouchard, R. Martini, M. Bernacki // *Journal of Materials Science* **48** (2013) 979.
[3] S.A. Kukushkin // *Journal of Applied Physics* **98** (2005) 033503.
[4] N.F. Morozov, I.A. Ovidko, Y.V. Petrov, A.G. Sheinerman // *Reviews of Advanced Materials Science* **4** (2003) 65.
[5] C.H. Tsai, C.S. Liou // *Journal of Manufacturing Science and Engineering* **125** (2003) 519.

[6] B.G. Gorshkov, A.S. Epifanov, A.A. Manenkov, A.A. Panov // *Quantum Electronics* ***9*** (1979) 1420.
[7] K. Nordlund, J. Keinonen, M. Ghaly, R.S. Averback // *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* **148** (1999) 74.
[8] A.A. Manenkov, A.M. Prokhorov // *Physics-Uspekhi* **29** (1986) 104.
[9] W.L. Chan, E. Chason // *Journal of Applied Physics* **101** (2007) 121301.
[10] H. Metiu, A.E. De Pristo // *Journal of Chemical Physics* **91** (1989) 2735.
[11] M. Ghaly, K. Nordlund, R. S. Averback // *Philosophical Magazine A 79* (1999) 795.
[12] F. Karetta, H. M. Urbassek // *Journal of Applied Physics* **71** (1992) 5410.
[13] S. Plimpton // *Journal of Computational Physics* **117** (1995) 1.
[14] A. Stukowski // *Modelling and Simulation in Materials Science and Engineering* **18** (2009) 015012.
[15] M. Solar, H. Meyer, C. Gauthier, O. Benzerara, R. Schirrer, J. Baschnagel // *Wear* **271** (2011) 2751.
[16] T.J. Maloney, J. Frey // *Journal of Applied Physics* **12** (1977) 781.
[17] B. Gelmont, K. Kim, M. Shur // *Journal of Applied Physics* **74** (1993) 1818.
[18] P. Wynblatt // *Journal of Physics and Chemistry of Solids* **29** (1968) 215.
[19] C.P. Flynn // *Physical Review* **171** (1968) 82.
[20] J.A. Van Vechten // *Physical Review B* **12** (1975) 1247.
[21] T. Kinoshita, T. Wenger, D.S. Weiss // *Nature* **440** (2006) 900.
[22] B.A. Danilchenko, T. Paszkiewicz, S. Wolski, A. Jezowski, T. Plackowski // *arXiv preprint* (2006) cond-mat/0604270.
[23] K.T. Regner, D.P. Sellan, Z. Su, C. H. Amon, A.J. McGaughey, J.A. Malen // *Nature Communications* **4** (2013) 1640.
[24] C.A. Ratsifaritana, P.G. Klemens // *International Journal of Thermophysics* **8** (198) 737.
[25] Y. Lee, S. Lee, G.S. Hwang // *Physical Review B* **83** (2011) 125202.
[26] P.G. Klemens // *Proceedings of the Physical Society. Section A* **68** (1955) 1113.
[27] W.W. Mullins, R.F. Sekerka // *Journal of Applied Physics* **34** (1963) 323.
[28] S.R. Coriell, R.L. Parker // *Journal of Applied Physics* **36** (1965) 632.
[29] S. R. Coriell, R.F. Sekerka // *Journal of Crystal Growth* **34** (1976) 157.
[30] R. Panat, K. J. Hsia, D.G. Cahill // *Journal of Applied Physics* **97** (2005) 013521.
[31] S.A. Kukushkin, A.V. Osipov, A.V. Redkov // *Physics of the Solid State* **56** (2014) 2530.
[32] A.V. Redkov, A.V. Osipov, S.A. Kukushkin // *Physics of the Solid State* **57** (2015) 2524.
[33] I.A. Ovidko, A.G. Sheinerman // *Reviews on Advanced Materials Science* **9** (2005) 17.
[34] R.J. Asaro, W.A. Tiller // *Metallurgical Transactions* **3** (1972) 1789.
[35] W.W. Mullins, R.F. Sekerka // *Journal of Applied Physics* **5** (1964) 444.