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Advanced mechanochemistry for solid state hydrogen storage Materials synthesis.

Polański Marek[1]

[1] *Military University of Technology, 2 Kaliskiego Street, Warsaw, 00-908, Poland*

Corresponding Author(s): marek.polanski@wat.edu.pl

Abstract: Reactive milling (or grinding) is one of the mechanochemical processes that uses common ball mills. Its goal is not only to refine and mill the input material but also to cause its reaction - typically with gas filling the working cylinder (for example, hydrogen). This process is frequently used to create complex hydrides, such as binary and ternary metal hydrides, which are considered as materials for hydrogen and heat storage. This method, which has been around for a long time, is widely used in hundreds of laboratories worldwide because it is simple to use and produces excellent results. The reaction is typically carried out using cylinders made of a material with high abrasion resistance and a grinding medium in the form of steel or ceramic balls for grinding the batch material in the version that is most commonly employed. The capabilities of the technique may be significantly extended by making its modifications in o-rder to fo-r example control the temperature of the milling process o-r by changing o-r even removing the grinding media. In this presentation, the unusual a-nd unobvious cases of mechanosynthesis of the solid-state hydrogen storage materials are shown a-nd described.

Keywords: hydrogen storage, mechanical alloying, reactive milling, ball milling.

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Fracture induced microstructure evolution at extremely low temperatures

Skoczeń Błażej[None]

One of the crucial problems related to application of metastable materials at extremely low temperatures is fracture. Until now fracture has been analyzed by means of classical approach based on the stress intensity factor or the J-integral. The classical models by Griffith, Irwin or Dugdale were used. However, initiation and propagation of macro-crack in metastable materials, like stainless steels, induces considerable evolution of the microstructure, that affects the conditions of fracture. In particular, the macrocrack propagation at the temperature of liquid nitrogen or liquid helium is accompanied by fast strain induced fcc-bcc phase transformation. The presence of secondary phase at the crack tip or along its trajectory alters the fracture conditions in two-phase continuum and has to be accounted for when predicting the lifetime of components. In order to investigate the phase transformation, the relevant constitutive model has been built. The experimental data were compared with the numerical simulations, including XFEM analysis.

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Martensitic transformation and phase stabilization in HEAs

Chulist Robert[1]

[1] *Institute of Metallurgy and Materials Science, Polish Academy of Sciences*

Corresponding Author(s): r.chulist@imim.pl

The phase transformation from face-centered cubic (fcc) to hexagonal close-packed (hcp) in the equiatomic CrCoNi medium- and CrMnFeCoNi high-entropy alloy has been investigated with diffraction of high-energy synchrotron radiation. The transformation has been induced by high pressure torsion at room and liquid nitrogen temperature by applying different hydrostatic pressures and shear strains. The hcp phase fraction after pressure release and heating-up to room temperature as a function of these parameters has been determined by Rietveld analysis. It increases with pressure and decreasing temperature. Depending on temperature a certain pressure is necessary to induce the phase transformation. The onset pressure depends on hydrostaticity; it is lowered by shear stresses. It is also lower for the medium-entropy alloy due to a lower stacking fault energy. The reverse transformation develops over a long period of time due to destabilization of the hcp phase. Moreover, the effect of the phase transformation on the microhardness of the HEA at room temperature will be demonstrated and discussed.

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Adsorption Mechanisms on Monolayer Graphenylene and their Effects on Optical and Electronic Properties

Francisco Javier Dominguez Gutierrez[1] ; Aligayev A. [2] ; Chourashiya M.[1] ; Papanikolaou S.[1] ; Huang Q.[2]

[1] *NOMATEN Centre of Excellence*

[2] *University of Science and Technology of China, Hefei, 230026, China*

Corresponding Author(s): javier.dominguez@ncbj.gov.pl, amil.aligayev@ncbj.gov.pl

Graphenylene (GPNL) is a two–dimensional carbon allotrope with a hexagonal lattice structure containing periodic pores. The unique arrangement of GPNL offers potential applications in electronics, optoelectronics, energy storage, and gas separation. Specifically, its advantageous electronic and optical properties, make it a promising candidate for hydrogen production and advanced electronic devices. In this study, we employ a computational chemistry–based modeling approach to investigate the adsorption mechanisms of CH_4 and CO_2 on monolayer GPNL, with a specific focus on their effects on optical adsorption and electrical transport properties at room temperature. To simulate the adsorption dynamics as closely as possible to experimental conditions, we utilize the self–consistent charge tight–binding density functional theory (SCC–DFTB). Through semi–classical molecular dynamics (MD) simulations, we observe the formation of H_2 molecules from the dissociation of CH_4 and the formation of CO+O species from carbon dioxide molecules. This provides insights into the adsorption and dispersion mechanisms of CH_4 and CO_2 on GPNL. Furthermore, we explore the impact of molecular
adsorption on optical absorption properties. Our results demonstrate that CH_4 and CH_2 affects drastically the optical adsorption of GPNL, while CO_2 does not significantly affect the optical properties of the two–dimensional material. To analyze electron transport, we employ the open–boundary non–equilibrium Green's function method. By studying the conductivity of GPNL and graphene under voltage bias up to 300 mV, we gain valuable insights into the electrical transport properties of GPNL under optical absorption conditions. The findings from our computational modeling approach might contribute to a deeper understanding of the potential applications of GPNL in hydrogen production and advanced electronic devices.

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DFT-based modelling of phase stability and properties of Cr-Ta-Ti-V-W high-entropy alloys

Wróbel Jan[1] ; Sobieraj D.[1] ; Goryaeva A. M.[2] ; Marinica M. -C.[2] ; Nguyen-Manh D.[3]

[1] *Faculty of Materials Science and Engineering, Warsaw University of Technology, Wołoska 141, 02-507 Warsaw, Poland*

[2] *Université Paris-Saclay, CEA, Service de Recherches de Métallurgie Physique, 91191, Gif-sur-Yvette, France*

[3] *CCFE, United Kingdom Atomic Energy Authority, Culham Science Centre, Abingdon, Oxfordshire, OX14 3DB, UK*

Corresponding Author(s): jan.wrobel@pw.edu.pl

High entropy alloys (HEAs) are the new class of materials incorporating four or more elements in similar concentrations. Due to their superior irradiation properties compared to pure elements and conventional alloys, HEAs are promising materials for applications in structural elements of future fusion and fission reactors [1].
In this work, the phase stability and properties of alloys in the Cr-Ta-Ti-V-W system are investigated using the combination of Density Functional Theory (DFT), Cluster Expansion (CE) method, Monte Carlo (MC) simulations, as well as Molecular Dynamics (MD) simulations using DFT-based Machine Learning (ML) potential. The analysis of chemical short-range order (SRO) parameters in Cr-Ta-Ti-V-W alloys obtained using DFT-based MC simulations shows that the most attractive interactions are observed for Cr-V and Ta-W pairs, however the chemical ordering depends significantly on temperature and the composition of alloy. It is shown that Ta-Ti-V-W alloys exhibit the lowest temperature of formation of disordered solid solution among all considered alloys [2].
In order to investigate the properties of Ta-Ti-V-W alloys, the accurate ML interatomic potentials [3] has been developed based on thousands of DFT calculations for the representative structures of alloys obtained using DFT-based MC simulations for different alloy compositions, different short-range ordering of structures and different classes of calculations: structure optimisations, calculations with applied strains, with a presence point defects, as well as ab initio MD simulations both for bcc and liquid phases. The root-mean-square errors between the forces computed using DFT and ML potential using the later approach are below 0.2 eV/Å. The developed ML potentials are applied in MD simulations in order to study the elastic and point defect properties, and melting temperatures of Ta-Ti-V-W alloys as a function of alloy composition.
[1] O. El-Atwani, N. Li, M. Li, A. Devaraj, J.K.S. Baldwin, M.M. Schneider, et al., Sci. Adv. 5 (2019) eaav2002.
[2] D. Sobieraj, J.S. Wróbel, T. Rygier, K.J. Kurzydłowski, O. El Atwani, A. Devaraj, et al., Phys. Chem. Chem. Phys. 22 (2020) 23929.
[3] A.M. Goryaeva, J. Dérès, C. Lapointe, P. Grigorev, T.D. Swinburne, J.R. Kermode, et al. Phys. Rev. Mater. 5 (2021) 103803.

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Chemical Segregation at the defect sinks in NiCo Based ODS-CSAs following high-temperature irradiation

Nori Sri T.[1] ; Vallum P. E.[2] ; Kalita D.[1] ; Chrominski W. [1] ; Zhang Y.[3] ; Kurpaska L. [1]

[1] *National Centre for Nuclear Research*

[2] *2Norwegian University of Science and Technology*

[3] *Idaho National Laboratory*

Corresponding Author(s): sri_tapaswi.nori@ncbj.gov.pl

In the past few years, oxide dispersion strengthened (ODS)-concentrated solid solution alloys (CSAs) emerged as potential structural materials for Gen. IV nuclear reactors. They can possess the best radiation resistance even at high temperatures (>400℃) as demonstrated in the limited studies conducted [1, 2]. One of the possible adverse effects of high-temperature irradiation is chemical segregation which can alter the stability of phases and local properties of the material. Hence, this work aims to examine this segregation phenomenon in some of the NiCo based ODS-CSAs.
The ODS-NiCoFe, ODS-NiCoFeCr, and ODS-NiCoCr were studied following Ni2+ irradiation at 580℃ and 700℃ via scanning transmission electron microscopy (STEM)-electron energy loss spectroscopy. The interfaces between the matrix and nanooxide particles and the grain boundaries act as defect sinks. Thus, these can be the regions of significant chemical redistribution during irradiation. Chemical segregation indicating Cr and Fe depletion and Ni and Co enrichment is expected near the grain boundaries specifically in Cr containing ODS-CSAs following irradiation. All such key findings which will culminate in evaluating the high-temperature radiation resistance of some of the ODS-CSAs will be presented.
[1] Y. Guo, M. Li, C. Chen, P. Li, W. Li, Q. Ji, Y. Zhang, and Y. Chang, Intermetallics, 117, 106674 (2020).
[2] C. Lu, M. Li, P. Xiu, X. Wang, G. Velisa, L. Jiang, K. L. More, J. D. Poplawsky, Y. Chang, Y. Zhang, and L. Wang, J. Nucl. Mater., 557, 153316 (2021).

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Application of stable isotopes of hydrogen and oxygen in materials science

Baron-Wiechec Aleksandra[1]

[1] *Department of Materials Science and Engineering, Guangdong Technion-Israel Institute of Technology (GTIIT), 241 Da Xue Road, Shantou, 515063, Guangdong, China.*

Stable isotopes, such as 18O, deuterium or 14C are very powerful species in probing materials to identify and to track ions diffusion under various environmental conditions. The isotopes acts as tracers and markers, which can be traced ex-situ by application of isotopic sensitive techniques. Isotopes are used in rather specific topics, for example in study of various aspects of materials performance in nuclear fission and fusion environments, in developing new materials for water splitting or energy storage, as well as in medicine for drugs discovery. The concept of markers or tracers in studying diffusion in solids, permeation phenomena or plastic deformation is known, however it is not widely used due to some practical challenges, which will be discussed in this work. There are wide assortment of techniques sensitive to detection of hydrogen and oxygen and their isotopes, for example Ion Beam Analysis (IBA), Secondary Ion Mass Spectrometry (SIMS), Imagine plating, and thermal mass spectrometry (TDS). All these methods have advantages and limitations in estimating the quantity or distribution of the isotopes in materials.
This paper aim to present practical application of isotope tracer/marker approach in combination with accelerator based techniques and mass spectrometry, highlight the unique features of the methodology and present to the listener other complementary techniques. The examples used here are limited to investigation of thin oxide films on light metals [1, 2], and Hydrogen retention in selected nuclear materials. Nevertheless the marker/tracer concept can be easy implemented to study other materials at the nanoscale [3,4].

[1] A. Baron-Wiechec, M.G. Burke, T. Hashimoto, H. Liu, P. Skeldon, G.E. Thompson, J.-J. Ganem, I. C. Vickridge, Tracer study of pore initiation in anodic alumina formed in phosphoric acid, Electrochimica Acta, 113, 302–312, 2013
[2] A. Baron-Wiechec, P. Skeldon, J. J. Ganem, I. C. Vickridge, and G. E. Thompson, Porous anodic alumina Growth in Borax Electrolyte, Journal of Electrochemical Society, 159, C583-C589; 2012,
[3] I.C. Vickridge, J.J. Ganem, I. Trimaille, J.-L. Cantin Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2005 Vol. 232; Iss. 1-4
[4] B. Xia, J. J. Ganem, E. Briand, S. Steydli, H. Tancrez, and I. Vickridge. "The carbon and hydrogen contents in ALD-grown ZnO films define a narrow ALD temperature window." Vacuum 190 (2021): 110289.

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Current trends in nanostructured TiO2 modifications for efficient photocatalytic and photoelectrochemical green hydrogen production

Ewa Wierzbicka[1]

[1] *Military University of Technology in Warsaw*

Corresponding Author(s): ewa.wierzbicka@wat.edu.pl

One strategy of sustainable hydrogen generation is based on photosensitive materials that can split water into hydrogen and oxygen using solar radiation. TiO2 is the benchmark semiconductor material applied for photocatalysis (PC) and photoelectrocatalysis (PEC). It can form various nanostructures such as nanopowders, and anodic nanotubes/nanoporous arrays, with many times higher surface area in comparison to bulk materials, that show great potential for further modifications. The most efficient and frequently used approach to TiO2 modification is coupling it with noble metal cocatalysts such as Pt. This modification brings much higher PEC and PC process efficiencies assigned

to several effects, such as Schottky barrier formation, surface plasmon resonance, or co-catalytic hydrogen absorption. On the other hand, noble-metal-free modification strategies such as sensitization with other semiconductors, or so-called material self-doping, are becoming increasingly popular. Here will be shown, how adequately designed modification of nanostructured titania can improve water-splitting performance.

8

A Universal Empirical Interatomic Potential

Ju Li[1]

[1] *Massachusetts Institute of Technology*

I will describe the recent invention of a robust universal machine learning interatomic potential that covers much of the periodic table. More than one thousand GPU years were used to generate the ab initio training data guided by active learning. Diverse test simulations have shown this machine learning potential has outstanding performance, with energy error significantly less than the chemical accuracy (1kcal/mol) for even chemically very complex systems. This universal potential can run over a million times faster than density functional theory (DFT) when dealing with several thousand atoms, and the latest release allows for more than 50,000 atoms of arbitrary combinations of 72 elements to be simulated together. One can use this empirical potential to study realistic microstructures such as extended defects with curvatures and their interactions, realistic phase transformations, plastic deformation and damage evolution, electrochemical interfaces, etc. [J. Materiomics 9 (2023) 447]

Bio: Prof. Ju Li has held faculty positions at the Ohio State University, the University of Pennsylvania, and is presently a chaired professor at MIT. His group investigates the mechanical, electrochemical and transport behaviors of materials as well as novel means of energy storage and conversion. Ju is a recipient of the 2005 Presidential Early Career Award for Scientists and Engineers, the 2006 Materials Research Society Outstanding Young Investigator Award, and the TR35 award from Technological Review. He was elected Fellow of the American Physical Society in 2014, a Fellow of the Materials Research Society in 2017 and a Fellow of AAAS in 2020. Li is the chief organizer of MIT A+B Applied Energy Symposia that aim to develop solutions to global climate change challenges with "A-Action before 2040" and "B-Beyond 2040" technologies.

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Ab initio Calculation of Phonon Limited Charge Carrier Mobility

Author(s): Payden Brown[1]

Co-author(s): Ju Li [1]

[1] *Massachusetts Institute of Technology*

Corresponding Author(s): paydenb@mit.edu

The exploration of novel ionizing radiation detectors relies on various atomic, electronic, and structural materials properties. Charge carrier mobility is vital to semiconductor radiation detector performance, however a lack of experimental mobility data for these exotic semiconductors demands the application of ab initio techniques. The technique chosen for this task accounts for large interactions between phonons and charge carriers at finite temperatures, allowing for accurate prediction of phonon limited charge carrier mobility over a range of temperatures. This talk will outline the technique (using Quantum Espresso, Wannier90, and PERTURBO software) and show results for various semiconductors with potential radiation detector applications. Additionally, results from

crystal structure prediction with universal neural network empirical potential will be briefly discussed. Crystal structure prediction (CSP) has played a vital role in computational materials discovery for its ability to explore unknown energy landscapes of chemical systems. Neural network potentials (NNPs) have opened the door for more efficient CSP and, with recently developed models, can reach the same level of accuracy as DFT. One such NNP is the PreFerred Potential (PFP), a universal NNP that can be applied to any combination of 72 elements. PFP was paired with our variable-composition CSP algorithm to explore diverse inorganic binary systems.

10

Breakthroughs in the discovery of new forms of boron

Nevill Gonzalez Szwacki[None]

Corresponding Author(s): gonz@fuw.edu.pl

In this talk will make a concise but complete review of the present understanding about the different forms that boron can adopt in all dimensions. To understand the significance of the discovery of 2D boron crystals, named borophenes, I will start with bulk boron and its 6 confirmed structures, out of about 20 reported, all of them made up from different arrangements of B_{12} icosahedral units directly connected or through additional atoms. I will also talk about planar and quasi-planar small all-boron clusters and continue with molecular allotropes of boron, fullerenes. The discussion continuous with 2D boron that can also adopt different structures. The story could not be complete without mentioning 1D forms of boron like nanotubes and nanowires. Finally, I will also discuss new possible directions of research in this exciting field and make a connection between structural properties and the present and future usage of boron allotropes.

7

Fe-based functional materials with structural inhomogeneity for dynamic loading applications

Krzysztof Muszka[1] ; Kamil Cichocki[1] ; Piotr Bała[1] ; Janusz Majta[1]

[1] *AGH University of Krakow*

Corresponding Author(s): majta@metal.agh.edu.pl, muszka@agh.edu.pl, cichocki@agh.edu.pl, pbala@agh.edu.pl

In the presentation, we will discuss the study of the effects of dynamic loading on the mechanical response of two groups of Fe-based alloys. The first part of the presentation will focus on the effect of strain rate on the mechanical response of the ultrafine-grained Nb-microalloyed steel, which was developed through severe plastic deformation. We will analyze this effect in terms of both microstructural and mechanical aspects.

Moving on to the second part, we will explore the influence of Mo content in the newly developed (CoNiFeMn)1-xMox high entropy alloy. This investigation will specifically address its susceptibility to twinning under various strain rates and temperatures, including both room temperature and cryogenic conditions.

6

Lattice Orientation Heterogeneity vs. Void Growth in Single Crystals

Katarzyna Kowalczyk-Gajewska[1]

[1] *Institute of Fundamental Technological Research, Polish Academy of Sciences*

Corresponding Author(s): kkowalcz@ippt.pan.pl

Description of the ductile failure phenomenon for single crystals of metallic materials deforming by slip and twinning is in its infancy as opposed to the well-grounded studies available for phenomenological material description. Metals, like hcp Mg or Zr, especially in the form of single crystals, are highly anisotropic solids and they are known to suffer from low ductility and fracture toughness. The goal of our studies is to better understand and describe the void growth failure mechanism under the condition of locally constraint plastic deformation within the crystallite, which may further help to reduce limitations hindering use of such alloys as structural elements. We focus on the mutual interaction between the void growth and refined microstructure formation related to the non-uniform lattice rotation due to presence of void and twinning activity. Using the proposed analytical/numerical approach the analysis of multiple factors influencing those phenomena will be performed, including overall loading scheme, local crystal orientation, initial porosity, and in particular twinning activity.

5

Healing of nano-cracks in metals due to internal stresses induced by microstructure evolution

T. Duong[1] ; A. Molkeri[2] ; C. M. Barr[1] ; A. Srivastava[2] ; K. Hattar[2] ; L. Boyce[1] ; M. J. Demkowicz[1]

[1] *Department of Materials Science and Engineering, Texas A&M University, College Station, TX 77843*

[2] *Center for Integrated Nanotechnologies, Sandia National Laboratory, Albuquerque, NM 87185*

Corresponding Author(s): demkowicz@tamu.edu

When external loads are applied to a material containing a crack, a characteristic stress field σ_{crack} builds up around the crack. If the material does not undergo any microstructure evolution during loading, the deflection of the crack faces depends on σ_{crack} alone. However, in polycrystalline metals, applied loads may cause the microstructure to evolve, e.g. through grain boundary migration, martensitic transformations, or differential distortion. This microstructural evolution generates complex stress fields σ_{mstr} of its own. The displacement of the crack faces then depends on the superposition of σ_{crack} and σ_{mstr}, rather than on σ_{crack} alone. This coupling between mechanically-driven microstructure evolution and internal stresses gives rise to counterintuitive crack behavior, such as closure under applied mode I (tensile) loading. This talk will present atomistic and continuum-level simulations of stresses induced at a triple junction during mechanically-driven grain boundary migration and their effect on the behavior of a nearby nano-scale crack. The simulations will be compared with corresponding experiments on fatigue-induced nano-cracks in polycrystalline Pt.

4

Designing Three-Dimensional Flat Bands in Topological Systems

Carmine Autieri[1]

[1] *Institute of Physics - PAN*

Corresponding Author(s): autieri@magtop.ifpan.edu.pl

Electrons with large kinetic energy have a superconducting instability for infinitesimal attractive interactions. Quenching the kinetic energy and creating a flat band renders an infinitesimal repulsive interaction the relevant perturbation. Thus, flat-band systems are an ideal platform to study the competition of superconductivity and magnetism and their possible coexistence. Recent advances

in the field of twisted bilayer graphene highlight this in the context of two-dimensional materials. Two dimensions, however, put severe restrictions on the stability of the low-temperature phases due to enhanced fluctuations. Only three-dimensional flat bands can solve the conundrum of combining the exotic flat-band phases with stable order existing at high temperatures. Here, we present a way to generate such flat bands through strain engineering in topological nodal-line semimetals. We present analytical and numerical evidence for this scenario and study the competition of the arising superconducting and magnetic orders as a function of externally controlled parameters. We show that the order parameter is rigid because the three-dimensional quantum geometry of the Bloch wave functions leads to a large superfluid stiffness in all three directions. Using density-functional theory and numerical tight-binding calculations, we further apply our theory to strained rhombohedral graphite and CaAgP materials.

3

Low and high temperature testing capabilities of Laboratory for Materials and Structures Testing

Kopec Mateusz[1]

[1] *Institute of Fundamental Technological Research Polish Academy of Sciences*

Corresponding Author(s): mkopec@ippt.pan.pl

Laboratory for Materials and Structures Testing of IPPT PAN offers mechanical testing under dynamic and static force, including standard methods for measurements of tensile and compression strength, impact resistance, bending, fracture toughness, fatigue, creep, biaxial testing and SHPB. We are able to perform most of these tests in wide range of temperature from -273℃ to 1000℃ and strain rates from 10^-5 to 10^4. Apart from destructive methods we are using ultrasonic and eddy currents methods as well as digital image correlation, optical and scanning electron microscopy. In this presentation, some low and high-temperature testing capabilities of the Laboratory for Materials and Structures Testing will be presented. On the one hand, a novel method for high-temperature fatigue strength assessment of nickel superalloy turbine blades under cyclic bending load at a temperature of 950℃ will be discussed. On the other, initial results for low-temperature testing of aluminium alloys in static and dynamic ranges will be shown.

2

Critical thickness and phase transition in thin layers grown on crystalline substrates

Paweł Dłużewski[1]

[1] *Institute of Fundamental Technological Research, Polish Academy of Sciences.*

Corresponding Author(s): pdluzew@ippt.pan.pl

The effect of threading dislocations as well as the effect of dislocations nucleated from the open surface of growing layer on the misfit dislocation formation are discussed. A brief overview of papers [1,2,3,4] which had a significant impact on mathematical prediction of the critical thickness for dislocation formation in thin layers is presented.

Also, we discuss prediction of various critical thicknesses which altogether limit a layer quality. The layer can be damaged by: (i) phase transition, (ii) fracture and/or (iii) misfit dislocations formation. Each of the phenomena mentioned corresponds to different critical layer thickness. In order to obtain a superlattice, e.g. multiplied quantum wells, of good quality none of the critical thicknesses should be overcome during the growth process.

The analysis concerns the prediction of phase transition phenomena [5] observed in:
(i) the layer deposited as the first one on a bulk crystal as well as
(ii) the layers deposited in a superlattice.

In the case of thin layers grown in a metastable regime the critical thicknesses of subsequently deposited layers differ significantly from each other. The capping of open layer changes the critical layer thicknesses too. In result, the misfit
dislocations formed at the bottom during the layer deposition can stand again up to the threading position after capping [1]. The consequences of such a mode of crystal growth for the resultant quality of thin layers are discussed in brief.

Literature
1. J. Matthews and A. Blakeslee, J. Cryst. Growth 27, 118–125 (1974).
2. L. B. Freund, J. Appl. Mech. 54, 553–557 (1987).
3. W. D. Nix, Metall. Trans. A 20, 2217–2245 (1989).
3. S. M. Hu, J. Appl.Phys. 69, 7901–7903 (1991).
4. A. Braun, K. M. Briggs, and P. Böni, J. Cryst. Growth 241, 231–234 (2002).
5. P. Dłużewski, J. Z. Domagala, S. Kret, D. Jarosz, M. Kryśko, and H. Teisseyre, J. Chem. Phys. 154, 154701 (2021).