Young Modulus and Microhardness of (Pb,Cd)Te Solid Solution Grown by SSVG and MBE Method

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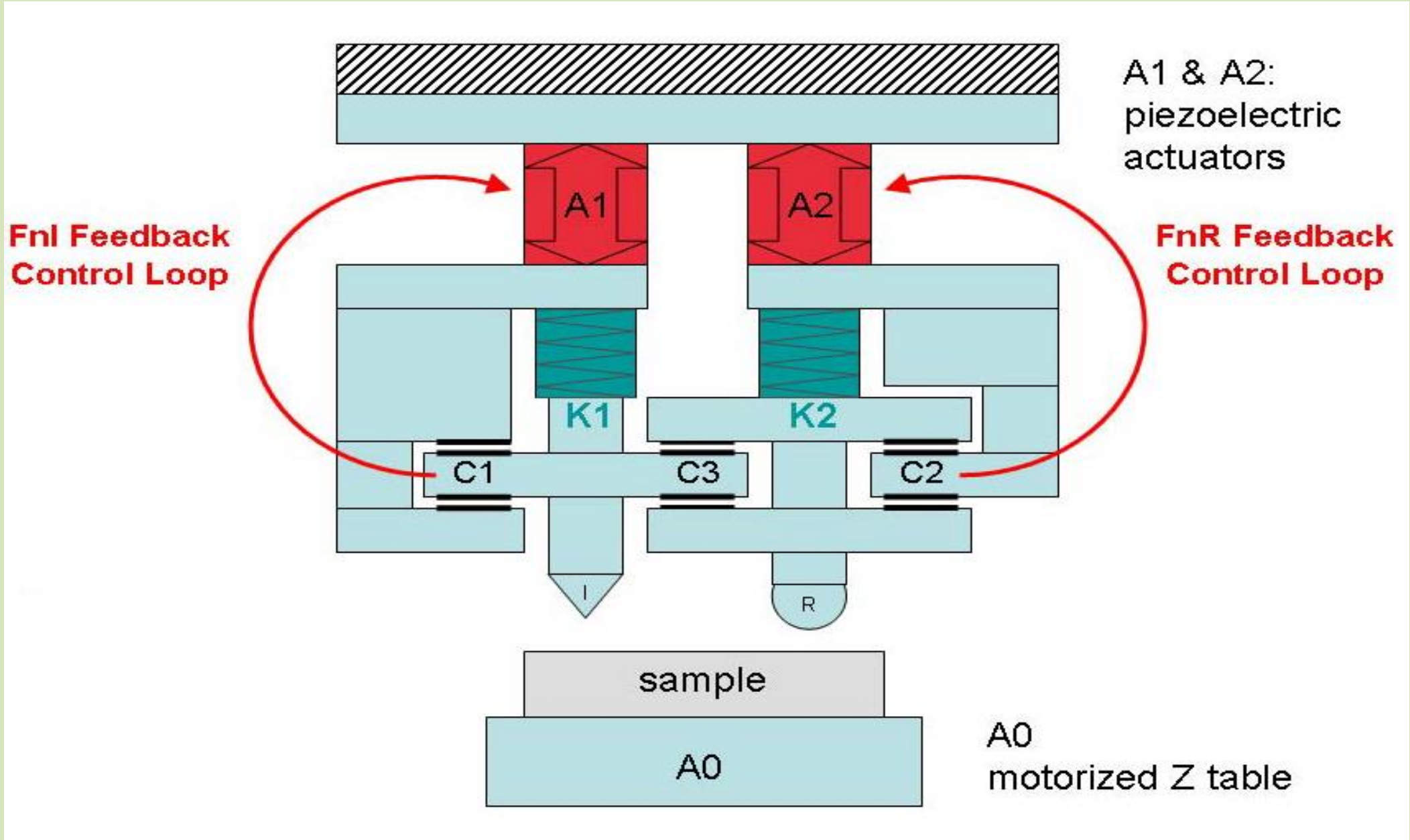
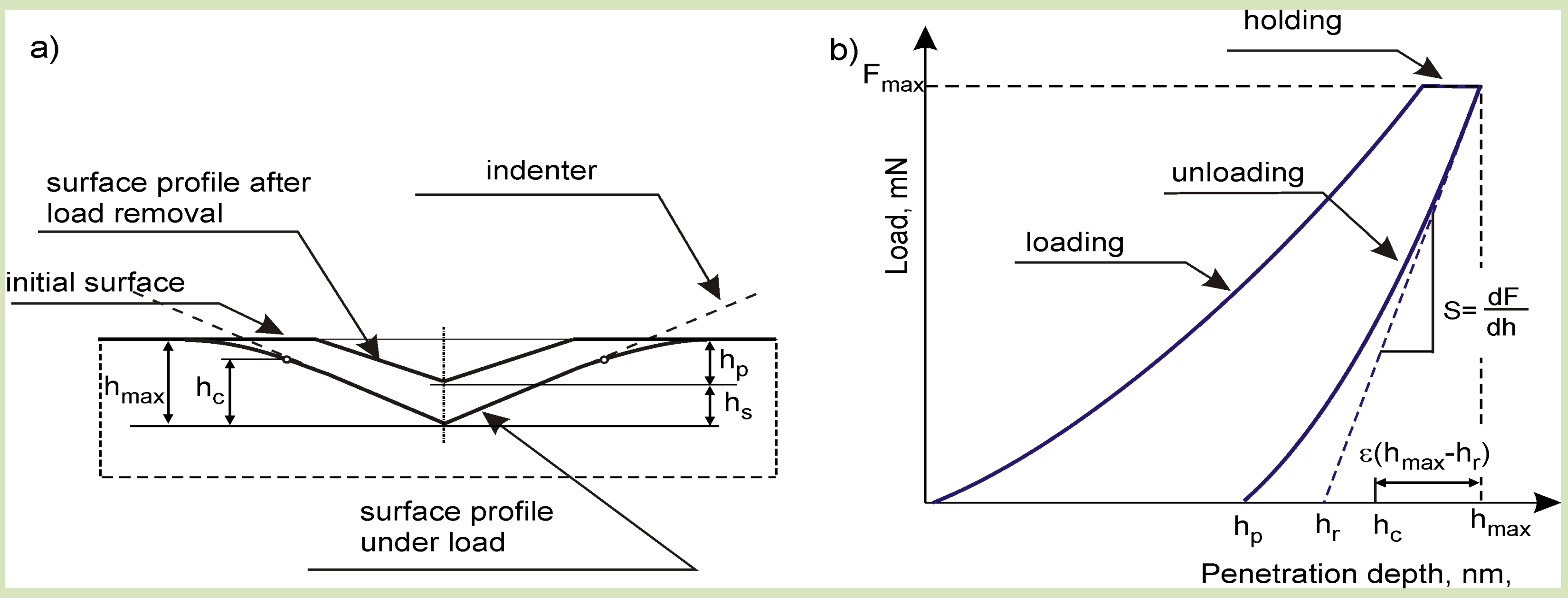
Motivation The PbTe, both alone or as a constituent of solid solutions, low-dimensional structures, composites etc., attracts an increasing interest due to the new physical findings, such as topological crystal insulators or dynamic local symmetry breaking and important applications, mostly in the harvesting energy area. A significant hardening of the (Pb,Cd)Te solid solution with an increasing CdTe content could be an attractive property for selected devices of such crystals (see, e.g. [1]). The aim of this work was to check a possibility to introduce Cd into PbTe by the MBE technique and to analyze resulting from it modification of selected mechanical properties of obtained materials.

Experiment Bulk, single (Pb,Cd)Te crystals containing up to a few percent of Cd were grown by the self-selecting vapor growth (SSVG) method [2]. The samples were characterized by XRD using X'Pert PANalytical diffractometer and Cu Kα_1 radiation. Two millimeter thick (001), (011) and (111)-oriented crystal plates were cut and etched using bromine-methanol solution. The microhardness and Young modulus for (001), (011) and (111)-oriented crystal planes were determined by the nanoindentation method.
The same mechanical properties of 2 micrometer thick, (100)-oriented MBE (Pb,Cd)Te layers, grown on GaAs substrate covered with 4 µm CdTe buffer layer were determined for a comparison. Before the growth substrates were etched in HCl in order to remove oxides and impurities. Samples were grown in 270°C using effusion cells of elemental Pb, Cd and Te with various flux ratio in order to achieve selected compositions of (Pb,Cd)Te solid solutions. The total Cd content in investigated layers was determined by EDX technique, solid solution composition was checked by XRD measurements.

Determination of microhardness (H) and Young modulus (E) by the nanoindentation



Two-axis UNHT principle: A1 and A2 are the piezo actuators used for the application of the active reference force (FnR) and the indenter normal force (FnI). The indentation depth of the indenter tip is directly measured via the differential capacitive sensor C3.



a) Schematic representation of the indenter - sample contact.

b) Analysis of load-depth curve:
h_p - permanent indentation depth, h_r - tangent indentation depth, h_c - contact depth of the indenter with the sample at F_{max}, h_{max} - maximum indentation depth, S - contact stiffness.

Hardness is a measure of how resistant solid matter is to various kinds of permanent shape change when a compressive force is applied. Hardness in general depends on the strength of chemical bonds, but the behavior of solid materials under applied force is more complex.

Young modulus (elastic modulus) – is a mechanical property of linear elastic solid materials. It defines the relationship between stress (force per unit area) and strain (proportional deformation) in a material.

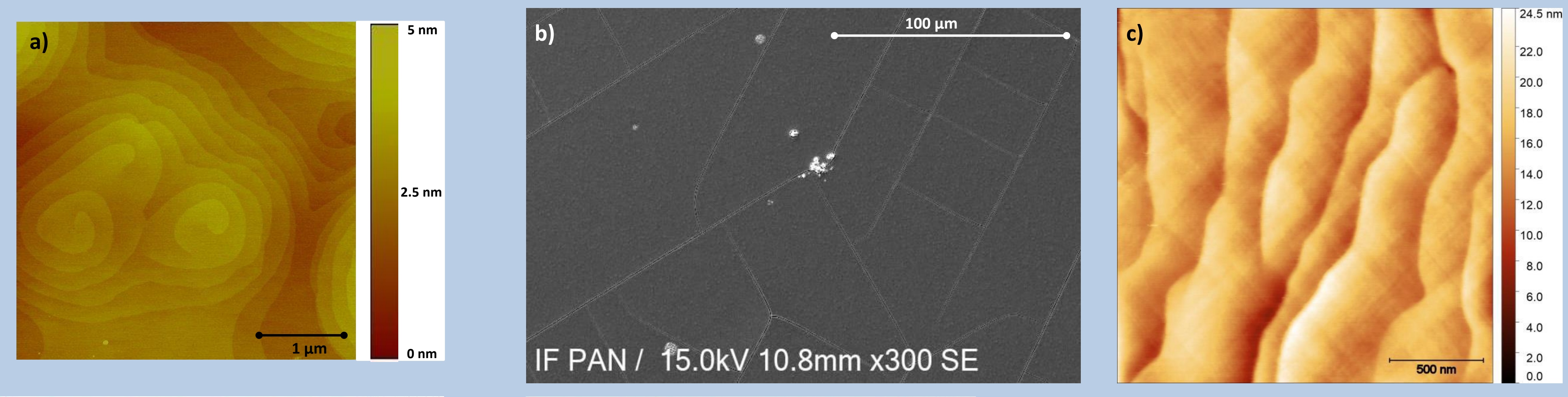
$$H = \frac{F_{\max}}{A_p}$$

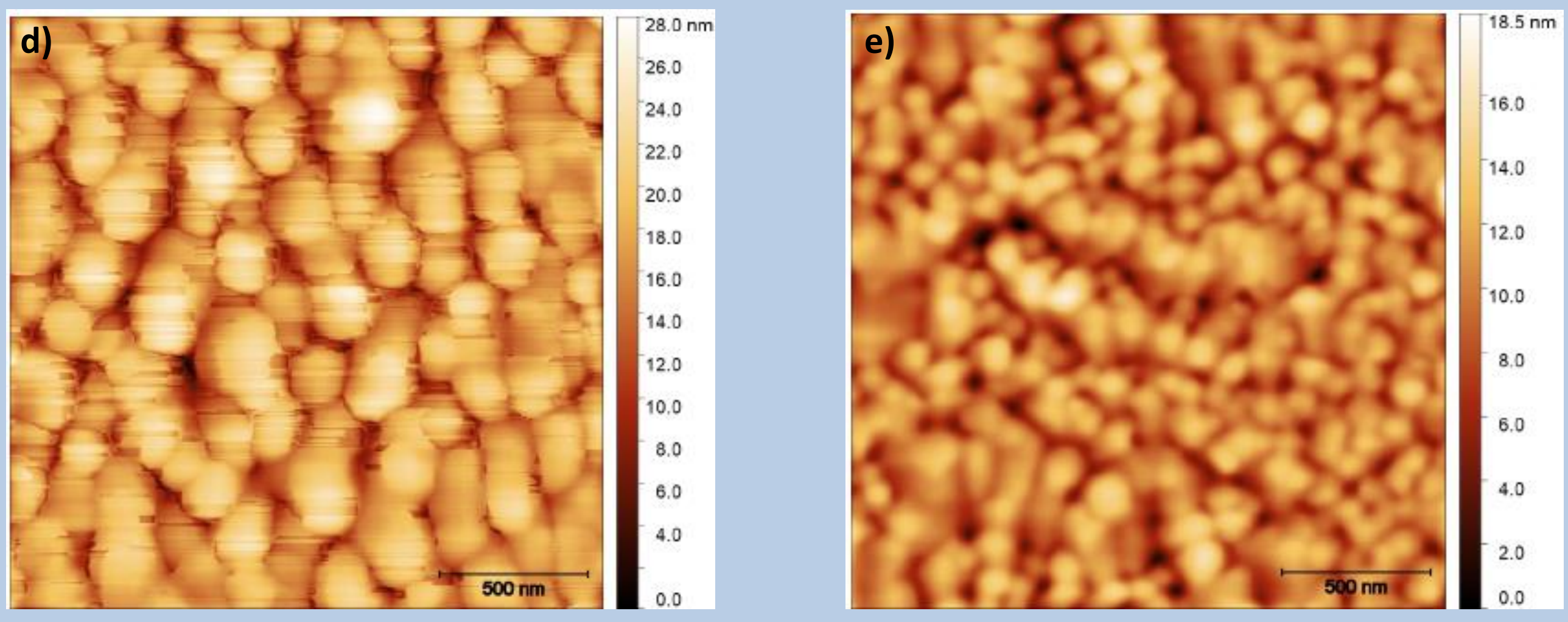
H- hardness, F_{max} - maximum test force, A_p - permanent indentation surface area

$$\frac{1}{E_r} = \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_s^2}{E_s}$$

where: E_r - reduced elastic modulus, E_i - elastic modulus of the indenter (diamond 1141 GPa), ν_i- Poisson's ratio of the indenter (diamond 0.07), E_s - elastic modulus of the specimen, ν_s - Poisson's ratio of the specimen.

Surface of (Pb,Cd)Te epitaxial layers



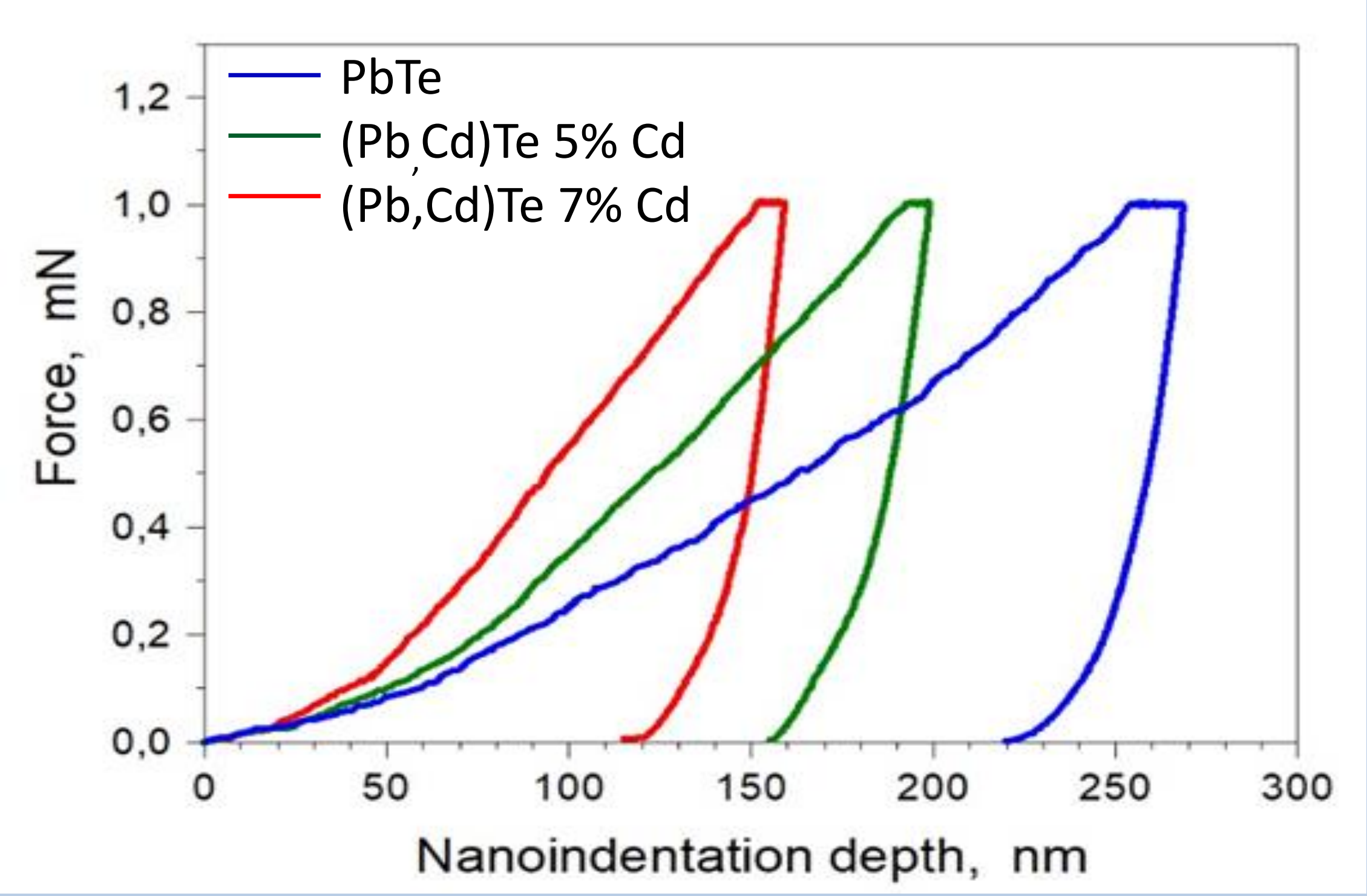


		RMS roughness [nm]
PbTe		2.5
(Pb,Cd)Te	5% Cd	3.6
(Pb,Cd)Te	7%Cd	2.3

AFM images: a) (111)-oriented PbTe on BaF$_2$, c) PbTe on CdTe/GaAs (100), d) (Pb,Cd)Te (5% Cd) on CdTe/GaAs (100), e) (Pb,Cd)Te (7% Cd) on CdTe/GaAs (100). b) SEM image: the surface of (100)-oriented sample grown on CdTe/GaAs substrate, cracs resulted from very different thermal expansion coefficients of the layer and the substrate. MBE-grown (Pb,Cd)Te layers show different morphology for various substrates and total Cd content.

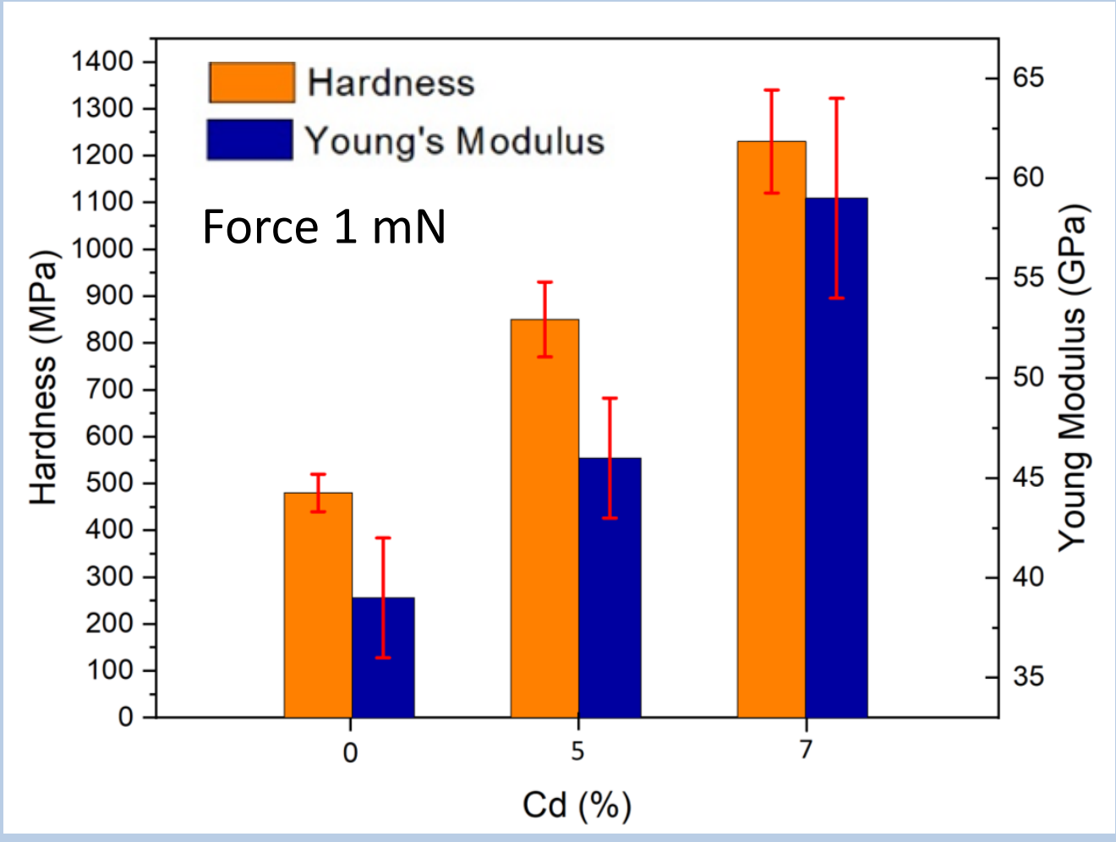
Microhardness and Young modulus for (100)-oriented (Pb,Cd)Te MBE layers

According to XRD data the highest amount of Cd which can replace Pb in (Pb,Cd)Te layer crystal lattice is close to 0.021. The presence of an additional Cd (occupying interstitial positions or forming small clusters) was confirmed by EDX measurements.



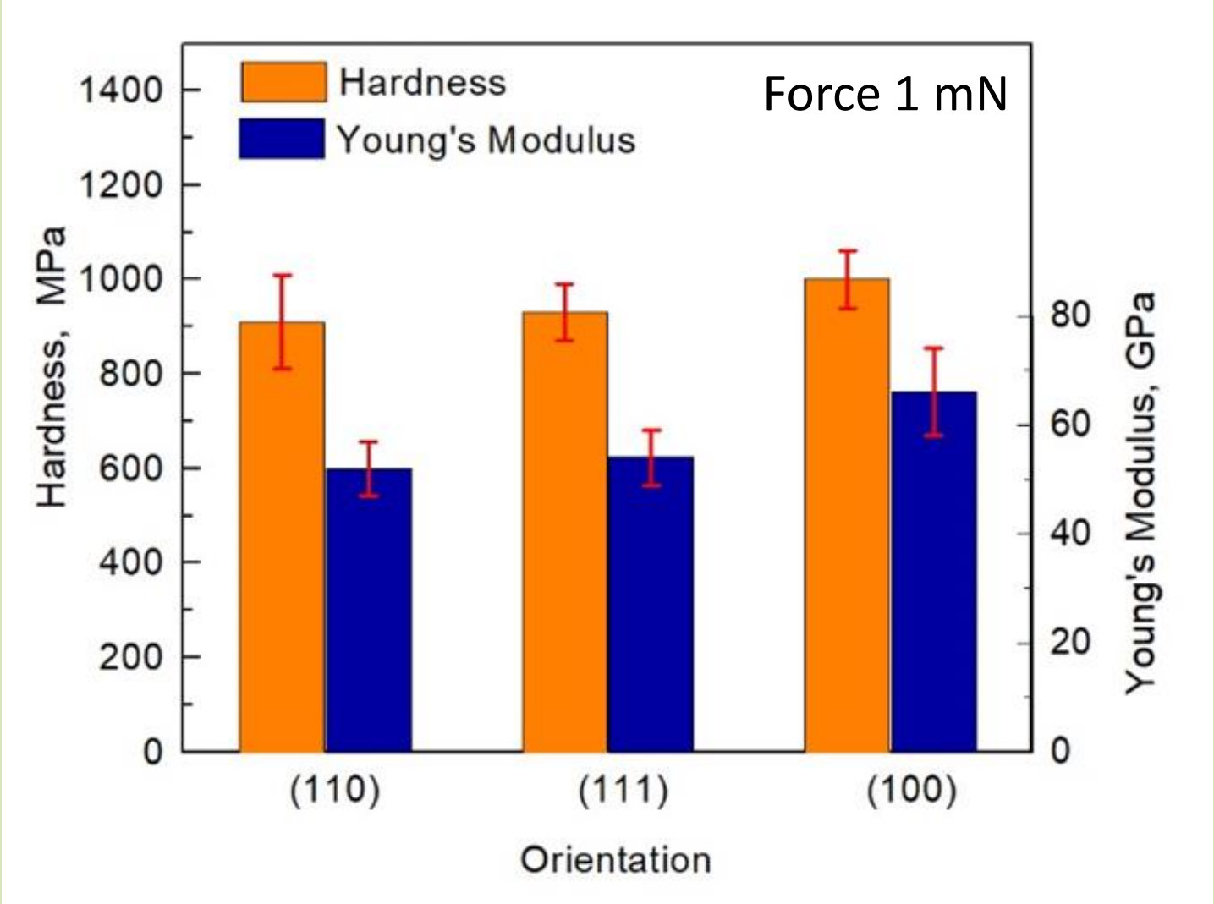
Nanoindentation experimental curves determined for (Pb,Cd)Te epitaxial layers with various total Cd content (0%, 5%, 7%). The maximum applied load was 1 mN.

Material		Hardness [MPa]	Young modulus [GPa]
GaAs		590±100	30±4
PbTe		480±40	39±3
(Pb,Cd)Te	5% Cd	850±80	46±3
	7% Cd	1230±110	59±5



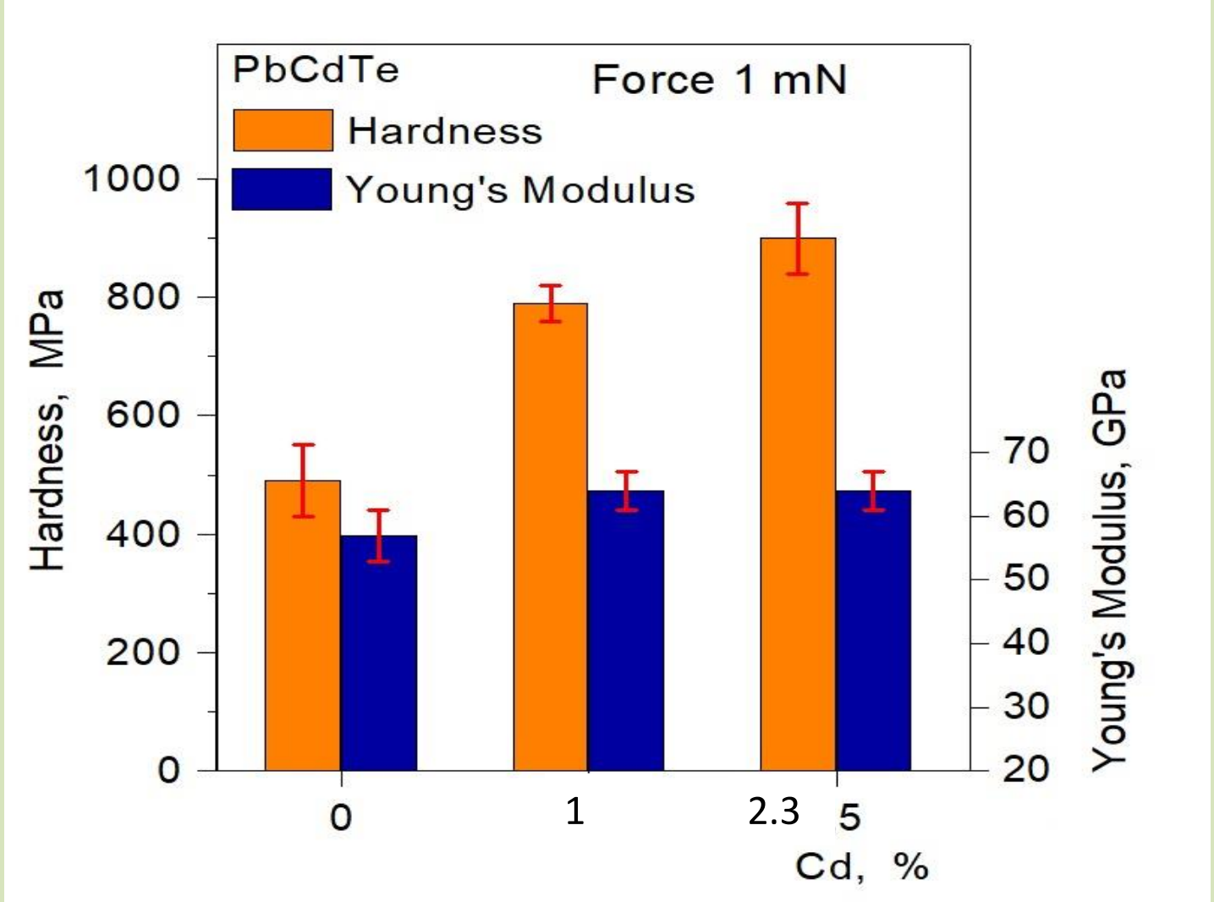
Young modulus and microhardness for (Pb,Cd)Te epitaxial layers as a function of total Cd content.

Microhardness and Young modulus for (Pb,Cd)Te bulk crystals



	(Pb,Cd)Te		
Orientaion	(100)	(111)	(110)
Hardness [MPa]	1000±60	930±60	910±100
Young modulus [GPa]	66±7	55±5	52±5

Microhardness and Young modulus for bulk (Pb,Cd)Te solid solution containing about 5% of Cd for various crystal orientations.



	Hardness [MPa]	Young modulus [GPa]
PbTe	490±60	57±4
(Pb,Cd)Te 1% Cd	790±30	64±3
(Pb,Cd)Te 2.3% Cd	900±60	64±3

Microhardness and Young modulus for bulk, (100) oriented (Pb,Cd)Te plates as a function of the solid solution composition.

Conclusions

The anisotropy of microhardness and Young modulus for (Pb,Cd)Te bulk crystals, determined by the nanoindentation reach the highest values for [001]-type direction which is in a qualitative agreement with our previous data for (Pb,Cd)Te solid solution [3] and theoretical predictions [4].
The surface quality of all (100)-oriented (Pb,Cd)Te layers grown on CdTe/GaAs substrates is not as good as that for (111)-oriented PbTe layer grown on BaF$_2$ substrate. Our results demonstrate that the upper limit of solid solution composition is close to 0.021 of Cd for (100)-oriented layers and an additional Cd does not occupy a substitutional site in the (Pb,Cd)Te crystal lattice. However, the microhardness of layers strongly depends on the total Cd content.

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