ТОМСКИЙ
ПОЛИТЕХНИЧЕСКИЙ
УНИВЕРСИТЕТ

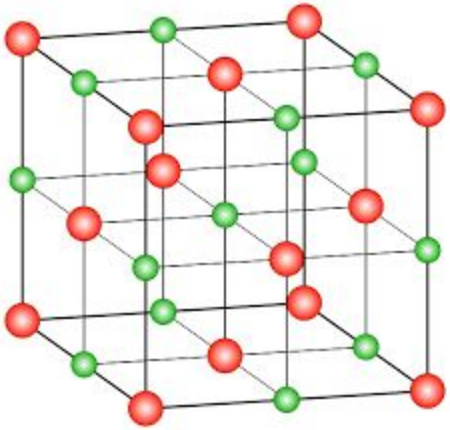
DEFECT IN SOLID

2017

What is a defect in a solid?

Solids consist of crystal. Crystals are described by scientists using an idealized model, but such crystals are not found in nature. The deviation of the crystal structure from the periodic crystal structure is defects. Crystals described by scientists using an idealized model, but such crystals are not found in nature.

The real crystal are not perfect. A real crystal always has a large number of imperfections in the lattice. One can reduce crystal defect considerably, but can never eliminate them entirely.



Model of perfect crystal

Defects are divided into four classes, if we consider the geometric of defects

- point defects
- Line defects
- Surface defects
- Volume defects

Defects occur in a solid at any temperature. The number of defects increases with increasing temperature and under the influence of ionizing radiation and mechanical treatment

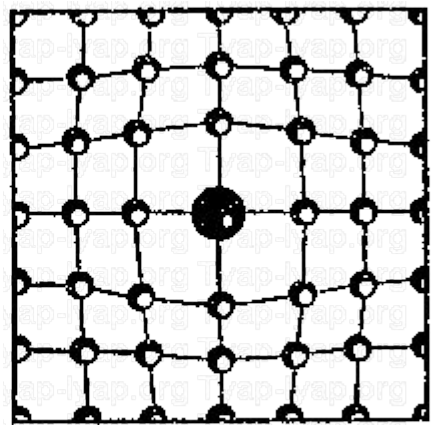
Point defects

To point defects include vacancies, atoms between the nodes of the crystal lattice, impurities.

Vacancy – An atom missing from regular lattice position. Vacancies are present invariably in all materials.

An impurity is a foreign atom that does not form a chemical compound in the crystal lattice

Point defect-vacancy



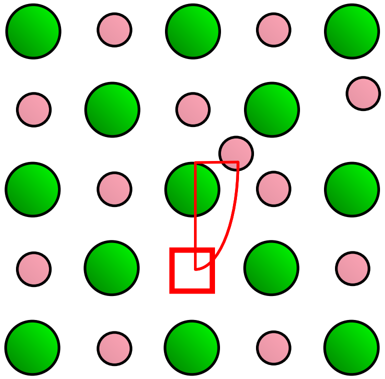
Point defect-impurity

Defect of Schotky and Frenkel

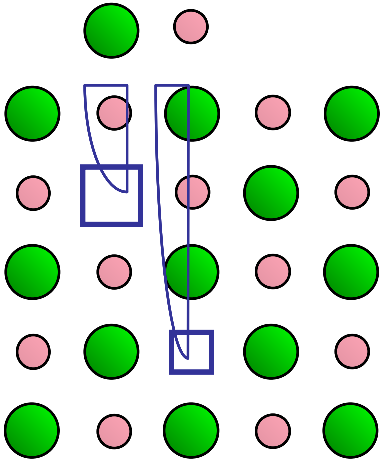
When the temperature is sufficiently high, as the atoms vibrate around their regular positions, some acquire enough energy to leave the site completely. When the regular atom leaves, a vacancy is created.

A pair of one cation and one anion can be missed from an ionic crystal. Such a pair of vacant ion sites is called ***Schotky defect.***

In crystals, an ion displaced from a regular site to an interstitial site is called **Frenkel** ***deffect***.



Frenkel defect: anion vacancy-interstitial cation pair



Schottky defect: anion -cation vacancy pair

Number of defect of Schotky

- The number of vacancies (defect of Shotky) is given by formula:

$$n = N \exp\left[-\frac{E_v}{k_B * T}\right]$$

- N-number of atom;
- n- number of vacancies;
- k_B- constant of Boltzman, $1{,}38*10^{-23}$ J /K;
- T- temperature of solid;
- E_v- energy of formation defect of Shotky;

Number of defect of Frenkel

- The number of defect of pair Frenkel is given by formula:

$$n = (N^{'}N)^{1/2}\exp\left[-\frac{E_f}{2k_B * T}\right]$$

- N-number of atom;
- N' - number of interstitial by can take up free atom;
- n- number of defects pair of Frenkel;
- k_B- constant of Boltzman, $1{,}38*10^{-23}$ J /K;
- T- temperature of solid;
- E_f- energy of formation pair of Frenkel.

Line defect- dislocation

- The experimental data do not show that the observed values of the yield strength are much smaller than the theoretical values. To explain this effect, a new two defect-dislocation.

  The two types of dislocations are:
- Edge dislocation
- Screw dislocation
- The experimental data do not show that the observed values of the yield strength are much smaller than the theoretical values. To explain this effect, a new type of defect- dislocation.

Результаты исследования

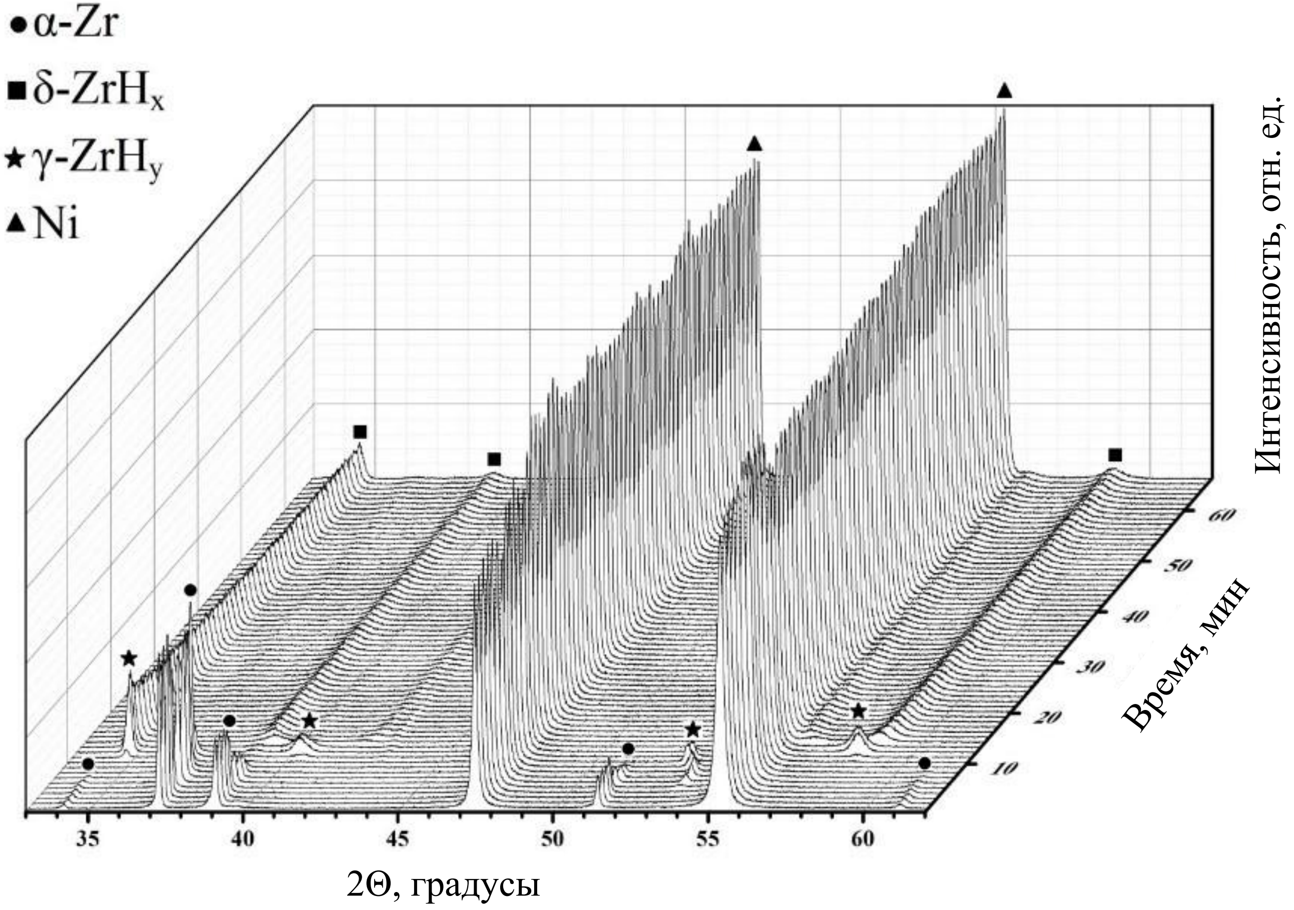


Рисунок 4 – Фазовые переходы в системе цирконий-водород с никелевым покрытием в процессе насыщения водородом при температуре 550 °C

Результаты исследования

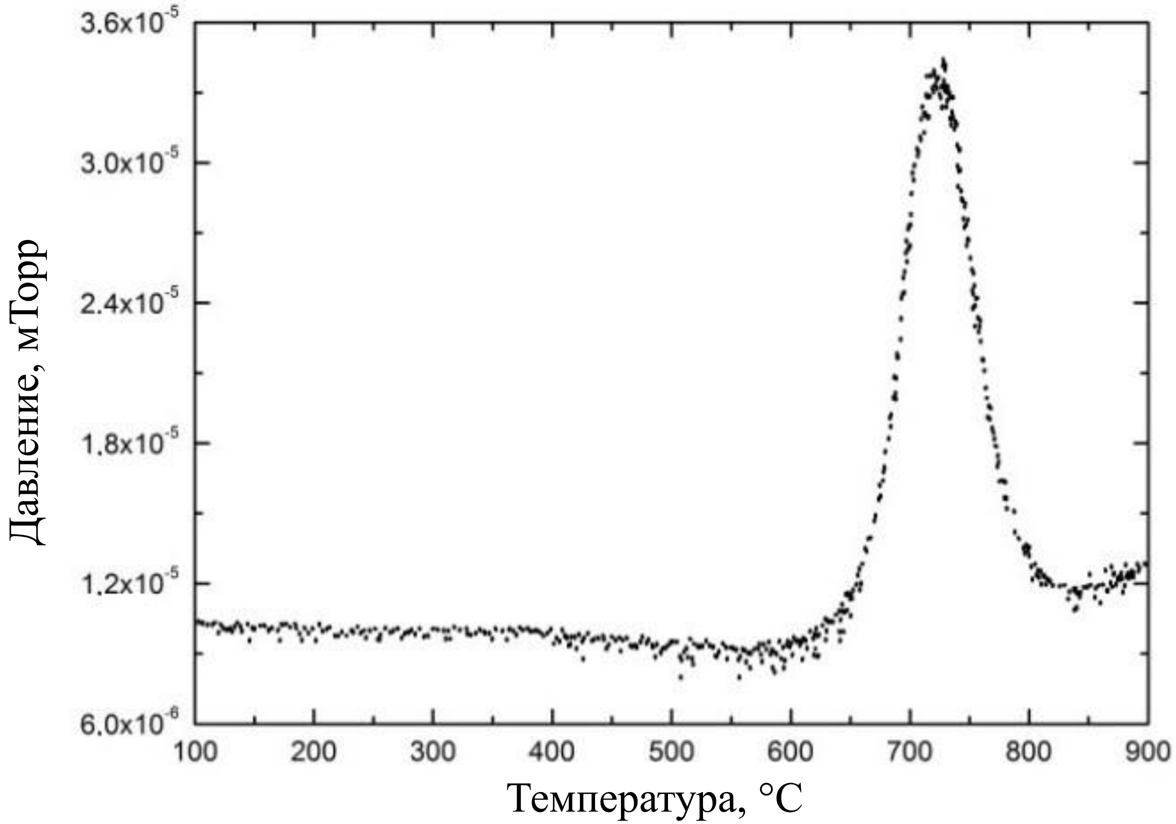


Рисунок 5 – Спектр термостимулированной десорбции водорода из образца циркониевого сплава после гидрирования в газовой атмосфере

Результаты исследований

Заключение

Исследовано взаимодействие водорода с циркониевым сплавом Zr1%Nb с нанесенным слоем никеля при газофазном гидрировании при температурах 350, 450 и 550 °C. Были сделаны следующие выводы:

- Скорость поглощения водорода циркониевым сплавом Э110 увеличивается в 16,8 раза при повышении температуры;
- При температуре 350 °C гидрирование приводит только к фазовому переходу α-циркония к δ-гидриду цирконию, тогда как при 450 и 550 °C процесс протекает с образованием метастабильной тетрагональной фазы гидрида циркония;
- При температуре 522-540 °C наблюдается процесс диссоциации гидридов в циркониевом сплаве Э110;
- При дальнейшем повышении температуры происходит увеличение β-фазы циркония из-за переходной фазы α → β циркония.

СПАСИБО
ЗА ВНИМАНИЕ!