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Claster model of N₂ – Ar, CO – Ar cryo alloys, comparative analysis

Cryocrystall solutions formed of linear molecules with atomic components are of considerable interest as convenient model systems. It is known that in some cases Vegard's rule and Prigogine theory are insufficient and in this connection novel approaches are needed. One of the deviations from an ideal solution manifests itself through the anomalous behavior of the lattice parameter as a function of the composition. For explanation of the unusual concentration dependence of the lattice parameter in CO₂ – Ar alloys the cluster model was used.

Key words: cluster model, cryogenic, electron diffraction.

Н.С. Мисько, В.В. Данчук, А.А. Солодовник

**Кластерная модель N₂ – Ar, CO – Ar
криогенных примесей, сравнительный анализ**

Растворы криокристаллов, образованные линейными молекулами с атомными компонентами, представляют особый интерес в качестве модельных систем. Для объяснения необычного эффекта зависимости параметра решетки от концентрации в сплавах CO₂ – Ar была использована кластерная модель, учитывающая не только изотропное взаимодействие между частицами, но также и наличие анизотропных сил в молекулярных матрицах. Методами электронной дифракции измерена зависимость параметра решетки от концентрации в системе азот-аргон при 20 К. Изучено влияние парных и тройных кластеров на параметры решетки раствора. Рассмотрены причины искажения, связанные с наличием кластеров в растворах N₂ – Ar, CO – Ar.

Ключевые слова: кластерная модель, криокристалл, электронная дифракция.

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**N₂ – Ar, CO – Ar криогенді қоспалардың кластерлік моделі,
салыстырмалы талдау.**

Атомды құраушылары бар сызықты молекулалардан түзілген криокристалдардың ерітінділері модельдік жүйе ретінде ерекше қызығушылық тудырады. Тор параметрінің CO₂ – Ar құймаларындағы концентрацияға тәуелділігінің ерекше эффектісін түсіндіру үшін бөлшектердің арасындағы изотропты әсерлесуді ғана емес, сонымен қатар молекулалық матрицалардағы анизотропты күштің болуын ескеретін кластерлік модель қолданылды. Электронды дифракция әдісімен 20 К температурада азот-аргон жүйесінде тор параметрінің концентрацияға тәуелділігі өлшенді. Жұптық және үштік кластерлердің ерітіндінің тор параметріне әсері зерттелді. N₂ – Ar, CO – Ar ерітінділерінде кластердің болуына байланысты қателердің себептері қарастырылды.

Түйін сөздер: кластерлік модель, криокристалл, электронды дифракция.

Cryocrystall solutions formed of linear molecules with atomic components are of considerable interest as convenient model systems. It is known that in some cases Vegard's rule and Prigogine theory are insufficient and in this connection novel approaches are needed. One of the deviations from an

ideal solution manifests itself through the anomalous behavior of the lattice parameter as a function of the composition. For explanation of the unusual concentration dependence of the lattice parameter in CO₂ – Ar alloys the cluster model was used. This semiquantitative theory takes into account not only

isotropic interaction between particles, but also the presence of anisotropic forces in the molecular matrices [1]. In recent study on the CO₂ – Kr solutions the theoretical analysis [2, 3] considering three mechanisms of interaction of Kr cluster with crystalline environment of CO₂ matrix was in a good agreement with the experiment. The possibility to study not only molecular matrix but and atomic may be realized in an investigation of nitrogen – rare gas alloys. According preliminary results [4] the theory describes well the behavior concentration dependence of the lattice parameter only for Kr in α – N₂. Additional experimental data are needed for N₂-Ar system. The comparison with CO-Ar alloy is interesting because this system is nearest analog. N₂ and CO have identical crystal structures, however the barriers which hinder the rotation of the molecules in an α – N₂ lattice are almost twice as small as in α – CO [5]. Observations were carried out in a stan-

dard electron diffractograph equipped with a helium cryostat. The deposition regime was chosen in order to obtain random distributions of impurity. The samples were grown *in situ* by depositing gaseous mixtures on Al substrate at T=20 K. The error in the lattice parameter measurements was usually 0.1%.

Detailed electron diffraction studies have been carried out for the nitrogen-argon system. The concentration dependence of the lattice parameter are measured at T=20 K for low concentrations. Using this data and obtained earlier [6] the relative lattice parameter change per unit impurity fraction is determined for investigated systems. The influence of pair and triple clusters on the lattice parameter of solutions has been studied. The distortion mechanisms related with the presence of clusters in the N₂-Ar, CO-Ar solutions are examined.

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