Surface composition of NiPd alloys

R. Noebe¹, J. Khalil¹,², G. Bozzolo¹,²

¹NASA Glenn Research Center, Cleveland, OH 44135, USA
²OAI, 22800 Cedar Point Rd., Cleveland, OH 44142, USA

Surface segregation in Ni-Pd alloys has been studied using the BFS method for alloys. Not only does the method predict an oscillatory segregation profile but it also indicates that the number of Pd-enriched surface planes can vary as a function of orientation. The segregation profiles were computed as a function of temperature, crystal face, and composition. Pd enrichment of the first layer is observed in (111) and (100) surfaces, and enrichment of the top two layers occurs for (110) surfaces. In all cases, the segregation profile shows oscillations that are actually related to weak ordering tendencies in the bulk. An atom-by-atom analysis was performed to identify the competing mechanisms leading to the observed surface behaviors. Large-scale atomistic simulations were also performed to investigate the temperature dependence of the segregation profiles as well as for analysis of the bulk structures. Finally, the observed surface behaviors are discussed in relation to the bulk phase structure of Ni-Pd alloys, which exhibit a tendency to weakly order.

Contact Information:
Email: Ronald.D.Noebegrnasa.gov
Phone: (216) 433-2093
CONCLUSIONS

A model was presented for describing surface properties of Ni-Pd alloys that not only reproduces existing experimental results but also provides a prediction for the observed enrichment observed in a Ni-Pd alloy. These results are consistent with the observed enrichment observed in a Ni-Pd alloy. The model assumes that the energy of formation of each cell of Ni-Pd alloys is given by

\[ \frac{1}{E_i} = \frac{1}{E_{Ni}} + \frac{1}{E_{Pd}} + \frac{1}{E_{Ni-Pd}} \]

where \( E_i \) is the energy of formation of each cell, \( E_{Ni} \) is the energy of formation of Ni, \( E_{Pd} \) is the energy of formation of Pd, and \( E_{Ni-Pd} \) is the energy of formation of Ni-Pd. The model suggests that the observed enrichment is due to the lower energy of formation of Ni-Pd compared to Ni and Pd.

The segregation behavior is explained by an atom-by-atom energetic analysis of Ni-Pd alloys. The model assumes that the energy of formation of each cell is given by

\[ \frac{1}{E_i} = \frac{1}{E_{Ni}} + \frac{1}{E_{Pd}} + \frac{1}{E_{Ni-Pd}} \]

where \( E_i \) is the energy of formation of each cell, \( E_{Ni} \) is the energy of formation of Ni, \( E_{Pd} \) is the energy of formation of Pd, and \( E_{Ni-Pd} \) is the energy of formation of Ni-Pd. The model suggests that the observed enrichment is due to the lower energy of formation of Ni-Pd compared to Ni and Pd.

The segregation behavior is explained by an atom-by-atom energetic analysis of Ni-Pd alloys. The model assumes that the energy of formation of each cell is given by

\[ \frac{1}{E_i} = \frac{1}{E_{Ni}} + \frac{1}{E_{Pd}} + \frac{1}{E_{Ni-Pd}} \]

where \( E_i \) is the energy of formation of each cell, \( E_{Ni} \) is the energy of formation of Ni, \( E_{Pd} \) is the energy of formation of Pd, and \( E_{Ni-Pd} \) is the energy of formation of Ni-Pd. The model suggests that the observed enrichment is due to the lower energy of formation of Ni-Pd compared to Ni and Pd.

The segregation behavior is explained by an atom-by-atom energetic analysis of Ni-Pd alloys. The model assumes that the energy of formation of each cell is given by

\[ \frac{1}{E_i} = \frac{1}{E_{Ni}} + \frac{1}{E_{Pd}} + \frac{1}{E_{Ni-Pd}} \]

where \( E_i \) is the energy of formation of each cell, \( E_{Ni} \) is the energy of formation of Ni, \( E_{Pd} \) is the energy of formation of Pd, and \( E_{Ni-Pd} \) is the energy of formation of Ni-Pd. The model suggests that the observed enrichment is due to the lower energy of formation of Ni-Pd compared to Ni and Pd.

The segregation behavior is explained by an atom-by-atom energetic analysis of Ni-Pd alloys. The model assumes that the energy of formation of each cell is given by

\[ \frac{1}{E_i} = \frac{1}{E_{Ni}} + \frac{1}{E_{Pd}} + \frac{1}{E_{Ni-Pd}} \]

where \( E_i \) is the energy of formation of each cell, \( E_{Ni} \) is the energy of formation of Ni, \( E_{Pd} \) is the energy of formation of Pd, and \( E_{Ni-Pd} \) is the energy of formation of Ni-Pd. The model suggests that the observed enrichment is due to the lower energy of formation of Ni-Pd compared to Ni and Pd.