# THERMODYNAMIC CHARACTERIZATION OF SHAPE MEMORY Al-Ni-Fe ALLOYS USING FACTSAGE

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# ABSTRACT

Shape memory alloys have again appealed a lot in recent years as new special materials of unusual macroscopic features that make them interesting for study and research as well as for their multifunctional application in various branches of techniques. Shape memory refers to the ability of certain plastic metals and alloys to regain their original shape during the heating process due to complete or almost complete absence of deformation. Shape memory effect has been studied for many alloys, as well as for some pure metals. In this paper the results of the thermodynamic characterization of Al-Ni-Fe alloys will be given.

Keywords: shape memory, thermodynamic, FactSage

### 1. INTORDUCTION

The shape memory effect had been noted as early as 1938, when Greninger and Mooradian [1] showed that the martensite phase in brass, an alloy of copper and zinc, could be made to form and disappear with a change in temperature. From that time to now, the essential step forward was done to understand the nature of shape memory alloys.

The effect of shape memory is ability of some metals and alloys deformed in martensite state or at temperature interval of martensitic transformation to regain their original shape during the heating process due to complete or almost complete absence of deformation [1, 2]. The heating process causes restoration of crystals in high-temperature phase, called beta or parent phase, and the removal of plastic deformation. In the same time, all physical and mechanical properties are restored.

During the shape recovering process, the alloys can produce a displacement or a force, or combination of the two as a function of temperature [2]. The starting force of recovering shape process is difference between free energies of parent and martensite phase during the reverse transformation. The complete shape recovering is only notice if the martensitic transformation is crystallography reverses and if the deformation process is done without plane shearing.

Shape memory effect has been studied for many alloys, as well as for some pure metals. However, investigations have shown that wide application can be found only for nitinol (Ni-Ti) and copperbased alloys that show shape memory effect. Copper-based alloys, compared to Ni-Ti alloys, possess somewhat lower mechanical properties due to their large grain size and elastic anisotropy. But, they can be improve, considerably without deterioration of shape memory effect, by small grain, method of rapid solidification, sinter metallurgy or by adding the elements such as: Zr, V, B, Ti, Cr, Fe, etc. [3].

In this paper will be given results of the thermodynamic characterization of shape memory ternary alloys Al-Ni-Fe system, which is a constituent of the system Cu-Al-Ni-based shape memory alloys.

#### 2. EXPERIMENTAL PART

The investigated shape memory alloys are obtained by classical method of melting in the induction furnace from pre-alloys Ni-Al and Ni-Fe, and casting into graphite modules, with hot and cold deformation to profiles of small cross sections.

Thermodynamics of the shape memory alloys Al-Ni-Fe have been done using FactSage [4]. The FactSage consists of a series of modules, which enable access to and manipulation of pure substances to the multi-component systems and alloys. The thermodynamics were done at temperature interval 1873-1973K.

### 3. RESULTS AND DISCUSSION

Chemical composition of obtained alloys with relationship Ni:Fe=7:3 is shown in Table 1. Values for the thermodynamic properties for the investigated alloys are given in Table 2.

Phase diagrams of the investigated systems of alloys obtained by FactSage are shown in Fig. 1-3. Comparison with referent data [5] indicate to fairly well accordance with available phase diagrams in literature.

| No | xAl | xNi  | xFe  |
|----|-----|------|------|
| 1  | 0   | 0,7  | 0,3  |
| 2  | 0,1 | 0,63 | 0,27 |
| 3  | 0,2 | 0,56 | 0,24 |
| 4  | 0,3 | 0,49 | 0,21 |
| 5  | 0,4 | 0,42 | 0,18 |
| 6  | 0,5 | 0,35 | 0,15 |
| 7  | 0,6 | 0,28 | 0,12 |
| 8  | 0,7 | 0,21 | 0,09 |
| 9  | 0,8 | 0,14 | 0,06 |
| 10 | 0,9 | 0,07 | 0,03 |
| 11 | 1   | 0    | 0    |

Table 1. Chemical composition of Al-Ni-Fe alloys.

Table 2. Results of thermodynamic characterization at 1973K.

| No. | aAl    | aNi    | aFe   | Gm Al              | Gm Ni   | Gm Fe  | ΔGm    | Gxs Al | Gxs Ni | Gxs Fe | ΔGxs   |  |
|-----|--------|--------|-------|--------------------|---------|--------|--------|--------|--------|--------|--------|--|
|     |        |        |       | Jmol <sup>-1</sup> |         |        |        |        |        |        |        |  |
| 1   | 0      | 0,660  | 0,250 |                    | -6794   | -22698 | -11565 |        | -944   | -2949  | -1545  |  |
| 2   | 0,0007 | 0,509  | 0,277 | -118680            | -11067  | -21044 | -24522 | -80909 | -3488  | 434    | -10171 |  |
| 3   | 0,003  | 0,331  | 0,290 | -91766             | -18115  | -20278 | -33364 | -65365 | -8604  | 3132   | -17140 |  |
| 4   | 0,014  | 0,180  | 0,270 | -69710             | -28106  | -21443 | -39188 | -49961 | -16405 | 4157   | -22154 |  |
| 5   | 0,044  | 0,082  | 0,216 | -50898             | -40989  | -25135 | -42099 | -35868 | -26759 | 2993   | -25047 |  |
| 6   | 0,117  | 0,031  | 0,144 | -35156             | -56570  | -31692 | -42132 | -23786 | -39349 | -572   | -25751 |  |
| 7   | 0,253  | 0,010  | 0,080 | -22494             | -74541  | -41309 | -39325 | -14115 | -53660 | -6529  | -24277 |  |
| 8   | 0,455  | 0,003  | 0,036 | -12898             | -94468  | -54150 | -33741 | -7048  | -68868 | -14651 | -20714 |  |
| 9   | 0,683  | 0,0008 | 0,013 | -6244              | -115921 | -70564 | -25458 | -2584  | -83670 | -24414 | -15246 |  |
| 10  | 0,875  | 0,0002 | 0,003 | -2188              | -139638 | -92359 | -14515 | -460   | -96017 | -34839 | -8180  |  |
| 11  | 1      | 0      | 0     | 0                  |         |        | 0      | 0      |        |        | 0      |  |







Figure 2. Phase diagram of Ni-Al system.



Figure 3. Phase diagram of Ni-Fe system.

Strong negative deviation from ideal behavior can be noticed for liquid Al-Ni-Fe shape memory alloys. The activities increase proportionally with increasing of the temperature. The activity and coefficient of activity values of the investigated components showed characteristics according to the Raoult's law. Considering calculated integral thermodynamic properties, all investigated alloys show negative values for integral Gibbs energy of mixing and integral excess Gibbs energy, except for the partial excess Gibbs energy for iron for alloys  $x_{Fe}$ =0.1-0.4.

## 4. CONCLUSION

The investigated shape memory Al-Ni-Fe alloys are obtained by classical method of melting in the induction furnace from pre-alloys, casting into graphite modules, with hot and cold deformation to profiles of small cross sections.

The thermodynamic properties of the investigated shape memory alloys at 1873K-1973K were determined.

Investigated system has negative values for integral excess and mixing Gibbs energy. Activity values of the components are less than unity and show negative deviation from the Raoult's law. The liquidus projection and the reaction scheme for the whole concentration range have been constructed, which are of interest for engineering applications, as well as for further basic materials researches.

### 5. ACKNOWLEDGEMENT

The financial support of the Ministry of Education and Science of the Republic of Serbia under the Projects TR 34005: "Development of ecological knowledge-based advanced materials and technologies for multifunctional application" and OI 172037: "Modern multi-component metal systems and nanostructured materials with different functional properties" is acknowledged.

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