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EFFECT OF RARE-EARTH IMPURITIES ON THE α - γ TRANSITION IN METALLIC Ce

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ABSTRACT:

The model of Ramirez and Falicov for α - γ transitions in pure Ce has been extended to describe Ce-rare earth dillute alloys. Predictions of changes in the transition temperatures and pressures are in good agreement with existing experiments.-

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In a recent letter (1) we have shown that a simple extension of the model proposed by Ramirez & Falicov (2) could account for a number of characteristics of the α - γ transition of Ce Th alloys such as the transition temperatures and pressures in going from the γ to the α phases and the disappeareance of first order transitions for Th concentrations above a certain critical value among others.

In this letter we wish to report similar calculations for alloys of Ce with other rare earths.

We assume that Eu and Yb remain divalent (4) while the other rare earths (with the exception of La) are trivalent when dissolved in Ce at all temperatures and pressures of interest (5).

Then, by the same procedure described in ref (1) we obtain the following expression for the free energy per atom of the alloys:

$$F = \frac{1}{2\alpha}\left[\bar{c}\,(4-n) + \eta\,\bar{x}\right]^2 + c\,\Delta\,n + c\,G\,n\left[\bar{c}\,(4-n) + \eta\,\bar{x}\right] +$$

$$+ x\,G\,(4-\eta)\left[\bar{c}\,(4-n) + \eta\,\bar{x}\right] + T\,c\left[\bar{n}\,\ell n\,n + (1-n)\,\ell n\,(1-n)\right] -$$

$$- T\,c\,n\,\ell n\,6 \qquad (1)$$

in temperature units ($k_B = 1$).-

c and x are respectively the Ce and rare earth concentrations in the alloy, while η is the valency of the rare earth impurity:

Two for Eu and Yb and three for the others. We have kept the same notation and values as used in ref. (1).

We may thus write the free energy per Ce atom in the form:

$$F = E\,n - \frac{B}{2}\,n^2 + T\left[\,n \ln n + (1 - n)\ln(1 - n) - n \ln 6\,\right] \qquad (2)$$

where

$$E = E_o - E_1\,x \qquad B = \left(2G - \frac{1}{\alpha}\right)(1 - x) \equiv B_o\,(1 - x)$$

$E_o = \Delta + 4\left(G - \frac{1}{\alpha}\right)$ is the distance from the Fermi level to the localized states and $E_1 = (4 - n)\,B_o$.

As shown in ref (1) the critical temperature is given by $T_c = B/4$ and the transition temperatures by $T_T = (E - B/2)/\ln 6$.

Choosing the pressure dependence of E_o so as to fit the transition temperatures for pure Ce and assuming that this is not affected by small impurity concentrations we obtain the phase diagrams shown in Fig (1). These show an increase of the transition pressures and a decrease of transition pemperatures in agreement with the general trend evidenced by the experiments of Gschneider et al (Ref. 3) for Pr, Dy and Lu.

The calculated transition temperatures for the 2% concentrations at zero pressure are $T_o^{3+} \approx 103$ °K for the trivalent impurities and $T_o^{2+} \approx 77$ °K for the divalent ones, in good agreement with the values reported by Meiner et al. (4), (6). For La the procedure used here would predict transition temperatures and pressures in contradiction with the results of both refs. (3) and (4), whether La were assumed to be a magnetic or non-magnetic impurity in Ce. In this respect it would be highly desirable to have direct experimental information (for instance such as provided by NMR) regarding possible changes in the occupation of the 4 f level of La in the range of temperatures and pressures not too far from the transition values.

In conclusion these calculations show that an extension of the R F model (described in ref 1) accounts clearly for the effect of the valency of the impurities in the phase diagram of Ce - rare earths alloys at low impurity concentracions. This provides additional support to the R F model.

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REFERENCES

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(3) K.A. Gschneidner,Jr, R.O. Elliot and R.R. McDonald, J. Phys. Chem. Sol 23, 1201 (1962)

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(5) If Eu becomes trivalent in the α phase and remains so when going back to the γ phase (4), the results are consistent with those of ref (4)

(6) We take T_o = 116 °K for pure Ce

FIGURE CAPTIONS

Fig. 1: Phase diagrams for Ce-rare earth alloys at low concentrations. Full line: pure Ce. Dashed line, trivalent impurities, Dot -dashed lines: divalent impurities. Dotted lines give the loci of Tc vs.pc for both cases. In Ce. R, R indicates rare earths generically. .

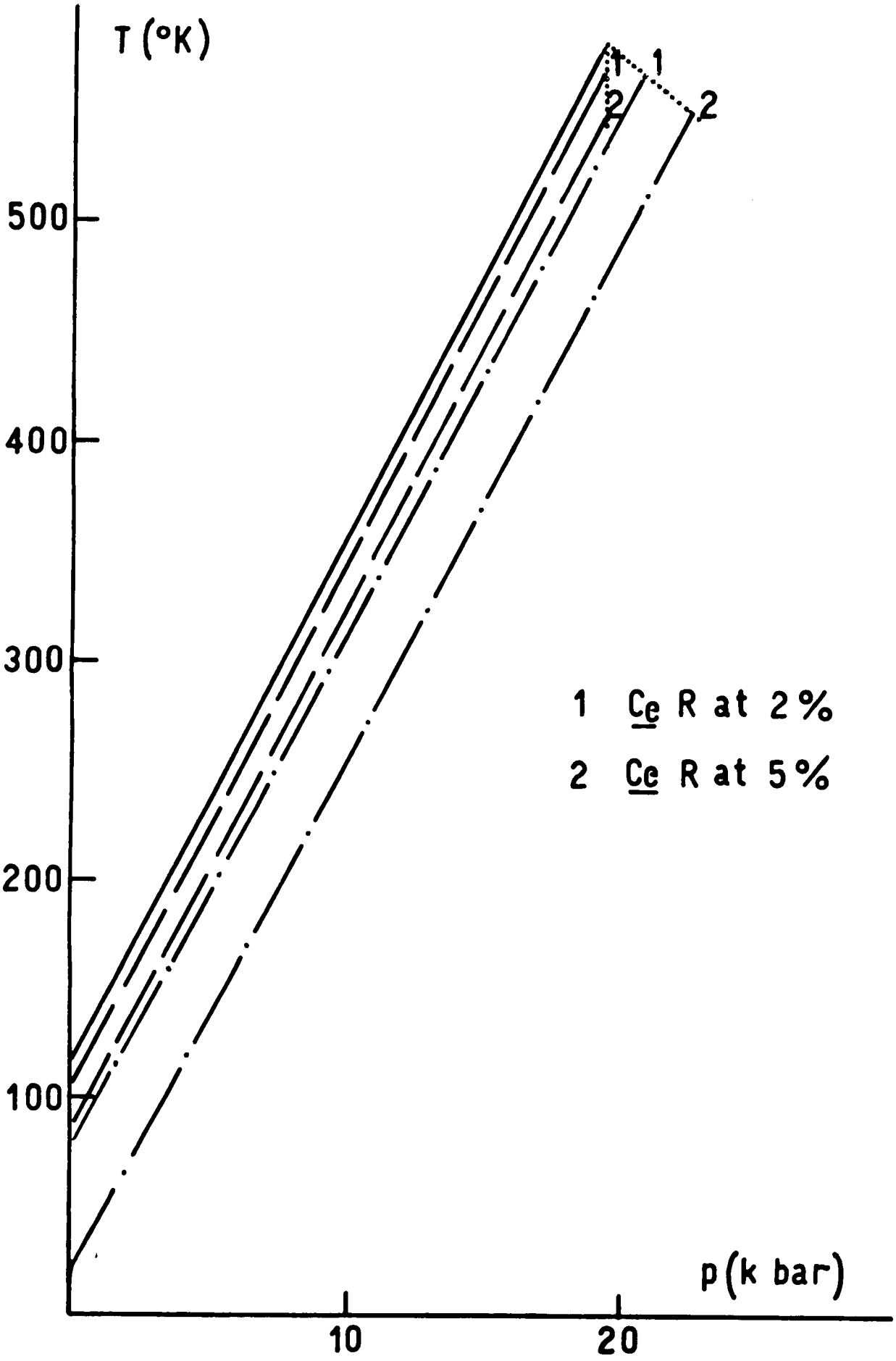

FIG. 1