PHYSICAL REVIEW B VOLUME

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X~=1 at. %, while Chelikowsky has used X,=0.5
at. %. To provide a finer distinction and at the
same time impose a more stringent test on the

model, we use X,=0.01 at. %. Furthermore, the
success of various solubility models also depends
critically on the temperature T, at which X,(T,) is measured. Early models ' often used data with T, at or above the solute melting temperature; Alonso and Simozar chose T, near the solute melting point, whereas Chelikowsky used T,=300 K. We
follow the latter

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TABLE I. Experimental solubilities in Be, Mg, Zn, Cd, Mg, and Si (Refs. 5 and 9—11), and the lattice location of
ion-implanted impurities in Be (Ref. 23) and Si (Ref. 24). The signs + and —denote soluble and insoluble elements,
respectively. The solubilities are taken from data at (or extrapolated to) room temperature T,=300 K for all solvents,
except Si and Ge for which the data is measured at T,=1250 and 900 K, respectively. For ion-implanted sites: S, sub-stitutional; 0, octahedral; T, tetrahedral; I, interstitial; R„random; D, defect association.

Impurity Be

Host

Mg Zn Cd Hg Si

Host

Impurity Be Mg Zn Cd Hg Si

Li
Na
K
Rb
Cs

CU

Ag
Au

Be
Mg
Ca
Sr
. Ba

Zn
Cd
Hg

B
Al
Ga
In
Tl

C
Si
Ge
Sn
Pb

0
S
Se
Te

0

S +
S +
S +

0

S
T

0

S,R
I +
0
T
0

0

0

I,R+
+ I
+
+ R
+ R

+
+

+ S,I—

+ I
+ I
S,I

S
+ +

+ S I+

+ S,I—
S,I

N
P
As
Sb
Bi

Sc
Y
La

T1
Zl
Hf

V
Nb
Ta

Cr
Mo
W

Mn
Tc
Re

Fe
Ru
Os

Co
Rh
Ir

Ni
Pd
pt

0
0
0—

+
T
T

R +
S

S,D+
S
S

I
Xe
Ne

0
0
I

R,S

Totals 23 38 29 22 37 24 19

B. Phenomenology of solid solubility

A number of phenomenological models have previously been attempted for predicting whether given elements will be soluble (to an extent X, at
temperature T,) in various host crystals. Largely,

these models are diagrammatic in nature. They are often based on the definition of dual coordinate

systems R ~(I,H) and R2(I,H), which defines two scales by which some chosen physical characteris-tics of the impurity (I) and host (H) are measured. One then attempts to find in the R ~(I,H) vs

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R2(I,H) plane for

a given host crystal two non-
overlapping and internally connected domains

corresponding to soluble and insoluble impurities. A successful choice of the scales R &(I,H) and
Rq(I, H) results in

a small number of misplaced
solutes (i.e.

, soluble element residing in the domain
of insoluble elements or vice versa) and can hence
be used as both

a systematizing and

a predictive
tool.

%e note that in solid-state physics and chemis-try there are numerous classical phenomenological models attempting to systematize predictively some

observed physical property S,b, (A,B) of binary AB systems in terms of general linear dual coordinate systems R&(A,B) and R2(A,B). One model is, for example, the Mooser-Pearson' model for classify-ing

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where RI '

represents the 12-coordinated
Goldschmidt radii, and Xl is the electronegativity

of the impurity atom I. Similarly, Chelikowsky
(C} has recently provided a separation of solid
solubilities using

Rc(I) «1/3

and (3)

R2 (I}=pl,

where $1 and nl*' are Miedema's parameters for the impurity elements.
Underlying the Darken-Gurry scheme are the
empirical Hume-Rothery' rules, which state that solid solubilities are encouraged by a small differ-
ence in atomic sizes between the solute and solvent

[i.e., ~ R & (I)—R &

(H) ~] and a sufficiently large
(but not too large) electronegativity difference [i.e., ~ Rq (I)—R2 (H) ~]. The first

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no systematic method that specifies the host-dependent ellipse (i.e.,

its origin and two radii and
the angle they make with the coordinate system). The ellipses are in fact drawn to include in them as many known soluble impurities as

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2.

0

SOLUBILITY IN Mg
Oibital Radii
Coordinates

Solubility

p 0.01%
4 Solubility

K0.01%

a,

Cs

valent hosts Mg (Fig. 4) and Zn (Fig. 5), for which the present model indicates,

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SOLUBILITY IN Cd
Orbital Radii Coordinates
SolubilityQ0. 01%
+ Solubility &0.01%

1.0

gSi

Ge
oLi

0.5
aTc

0.0
0.25 0.5

R~ {a.u.}
FIG. 6. Orbital-radii solubility map for Cd. The
data is taken at (or extrapolated to) T, =300 K (Refs. 5, 9, and 10).

have sketched simple elliptical domains which in-clude the most so1uble impurities. The overall rate of "success" of the orbital-radii coordinates [Eq. (1)] over this data base of 192 data points is simi-lar to that obtained by the empirical Miedema scale: 84%, compared with 82% using Miedema's parameters [Eq. (3)]. Given the fact that the present orbital-radii coordinates are, however, de-rived from first-principles and exclusively

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2.0

SOLUB
Orbital

Solu jSOIU
1.5

Sb

0.5

0.0
0.25

Mo

AujNi
Ti~

jlljTj
Mn —Cd
y

Ag
OaCr

0.5

I

0.75

I

1.0

R~ {a.u.}

FIG. 7 Orbital-radii solubility map for Hg. The data is taken at (or extrapolated to} T, =300 K (Refs. 5, 9, and 10).

dified parameters, one finds that Al and Cd are
also misplaced

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TABLE III. Reliability of various phenomenological
coordinates in predicting the location of ion-implanted
impurities in Si. The total number of implants is 26.

Scheme

Substitutional

(%)

Nonsubstitutional

(%)

Orbital radii
Miedema

Darken-Gurry'
Darken-Gurry

100
83
100
22

100
75
29
50

'Sood's criteria.
"Burne-Rothery criteria.

A comparison reveals that OR affects

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3.0

~ 2.0

5$

0
~ 1.0

P.Q

IMPLANTATION Si
Orbital

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TABLE V. Experimental (Ref. 24) data and various predictions for the ion-implantation site in Si. The symbols are
I, interstitial; S, substitutional; R, random; TI, tetrahedral interstitial. %henever experiment or theory shows a border-line case, both neighboring configurations are indicated. For comparison, we also show the solubility data (Ref. 11) at 950'C.

Impurity

Site: ion
implantation
(Ref. 24)

Experimental
Site: equilibrium
data

(Refs. 25—28)

Solubility
(Ref. 11)

OR

Eq. (1)

Miedema

Eq. (3)

Predictions

Darken-Gurry [Eq. (2)]
DG criteria Sood's criteria

Li
Na

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Vijay A. Singh, C. Weigel, L. M. Roth, and J. W. Corbett, Phys. Status Solidi B 100, 533 (1980).
Gold has been recently studied as a diffused impurity in Si [e.g., D. V. Lang, H. G. Grimmeiss, E. Meiger, and M. Jaros, Phys. Rev. B 22, 3917 (1980)]. It is certainly not substitutional.
From a recent EPR experiment, Troxell and Watkins [J.R. Troxell and G. D. Watkins, Phys. Rev. B 22, 921 (1980)] concluded that the natural boron impurity is metastable in Si, whereas the

thablteTj ET BT /Xi15 8.9 Tf 253.6

Vijay5ET BT /oodbur/Xi15 7.81 Tf 221.963637.0319 91(198ET BT BT /i15 8.75 Tf 140.44 636.434d (Z(198ET BT BT /i15 7.93 Tf 152.667678.336d (N Tj ET BT /(AcademicXi15 7.81 Tf 221.81 679.4364d (Gold) ET BT /Xi15 8.68 Tf 241.98 636.43 Td1(a)Tj ET BT /BT /Xi15 8.63 Tf 267.365 BT /471 5(diffu4ET BT 1962)Xi15 8.63 Tf 267 V. TI)i15 8.07 Tf 129.17 583.44 Td68in