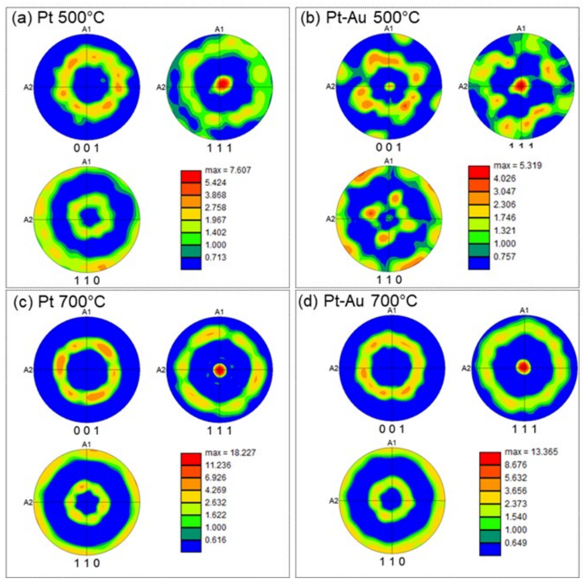
Electronic Supplementary Material (ESI) for Nanoscale.

The role of grain boundary character in solute segregation and thermal stability of nanocrystalline Pt-Au

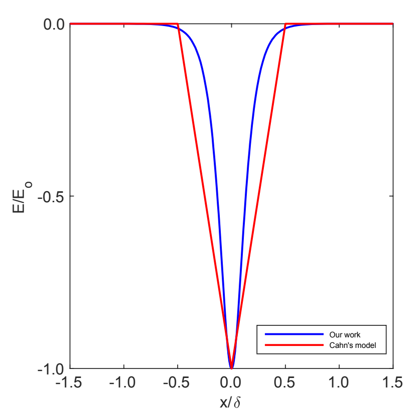
Electronic supplementary information

Christopher M. Barr[1], Stephen M. Foiles[1], Malek Alkayyali[2], Yasir Mahmood[2], Patrick M. Price[1], David P. Adams[1], Brad L. Boyce[1], Fadi Abdeljawad[2,3,*], Khalid Hattar[1,*]

1) Material, Physical, and Chemical Sciences Center, Sandia National Laboratories, Albuquerque, New Mexico, 87185, USA
2) Department of Mechanical Engineering, Clemson University, Clemson, South Carolina, 29634, USA
3) Department of Materials Science and Engineering, Clemson University, Clemson, South Carolina, 29634, USA



Supplemental Figure 1: Pole figures for (a, c) Pt and (b, d) Pt-10Au after the 500°C and 700°C anneals, respectively.



Supplemental Figure 2: The interaction energy function E(x) used in our work (blue) and the one used in Cahn's solute drag model (red).

Derivation of Cahn's Solute Drag Model

Our starting point is the governing differential equation for concentration profiles under steady-state GB migration with a velocity V, i.e., Eq. 6 in Cahn's solute drag model [42]

$$D\frac{\partial^2 c}{\partial x^2} + \frac{\partial c}{\partial x}\left[\frac{\partial D}{\partial x} + \frac{D}{RT}\frac{\partial E}{\partial x} + V\right] + \frac{c}{RT}\left[\frac{\partial D}{\partial x}\frac{\partial E}{\partial x} + D\frac{\partial^2 E}{\partial x^2}\right] = 0.$$

The above equation can be written in complete form as follows:

$$\frac{\partial}{\partial x}\left[D\left(\frac{\partial c}{\partial x} + \frac{c}{RT}\frac{\partial E}{\partial x}\right)\right] + V\frac{\partial c}{\partial x} = 0,$$

which can be solved by direct integration to yield the following for the first solution of the concentration governing equation.

$$c(x) = c_o e^{\left[\frac{-E}{RT} - \int_{x_o}^{x}\{V/D(\eta)\}d\eta\right]},$$

Now, the second solution for the concentration profile $c_2(x)$ can be obtained by the reduction of order method. First, we assume $c_2(x) = w(x)\, c(x)$, where $w(x)$ is to be determined. Next, we insert the ansatz for $c_2(x)$ in the governing differential equation for the concentration field to obtain, after some algebra:

$$Dc\frac{d^2 w}{dx^2} + 2D\frac{dc}{dx}\frac{dw}{dx} + c\frac{dw}{dx}\left[\frac{dD}{dx} + \frac{D}{RT}\frac{dE}{dx} + V\right] = 0.$$

The above can be written as:

$$\frac{d^2 w}{dx^2} + \frac{dw}{dx}\left[2\frac{1}{c}\frac{dc}{dx} + \frac{1}{D}\frac{dD}{dx} + \frac{1}{RT}\frac{dE}{dx} + \frac{V}{D}\right] = 0.$$

And noting that $D = D(x)$. The above equation can be integrated once using the substitution $z = \frac{\partial w}{\partial x}$ leading to

$$\frac{dz}{dx} = -\left[2\frac{1}{c}\frac{\partial c}{\partial x} + \frac{1}{D}\frac{\partial D}{\partial x} + \frac{1}{RT}\frac{\partial E}{\partial x} + \frac{V}{D}\right]z,$$

Which can be solved by direct integration

$$z = \frac{\partial w}{\partial x} = \frac{e^{\left[-\frac{E}{RT} - \int\left\{\frac{V}{D(\eta)}\right\}d\eta\right]}}{Dc^2}.$$

The above equation can be integrated once more to obtain the function $w(x)$ as

$$w(x) = \int_{-\infty}^{x} \frac{e^{\left[\frac{E}{RT} + \int\left\{\frac{V}{D(\eta)}\right\}d\eta\right]}}{D} d\xi.$$

Finally, $w(x)$ can be inserted into the ansatz for $c_2(x)$, which with c(x) provides the total solution for the concentration profile across a migrating GB with solute segregation.