
بسم الله الرحمن الرحيم

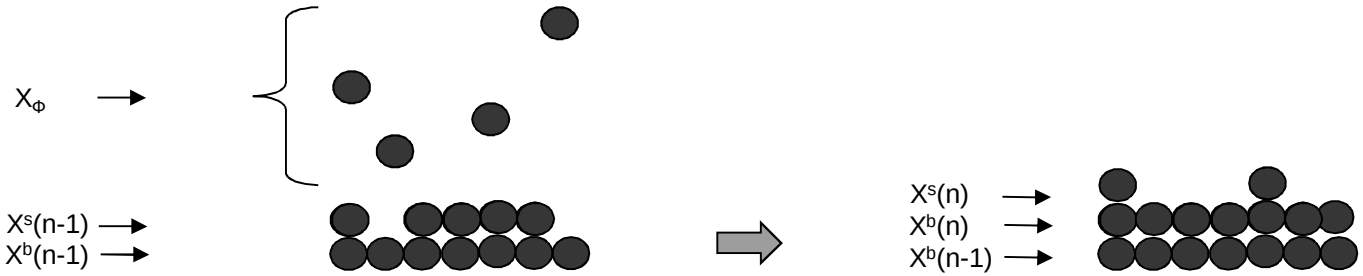
2) Kinetic Model

(Single-atom Segregation Model)

Segregation Energy

- Surface and bulk atoms: Let's define the "surface" atoms as the atoms in the last ML grown and "bulk" atoms, the atoms in only layer below the surface.
- Let's assume "X_Φ" is the nominal mole fraction in the incident flux and $X^s(n-1)$ is the concentration of atoms before "X_Φ" heads the surface.
- If $X^s(n)$ and $X^b(n)$ are the concentration of atoms in the layer "n" (after "X_Φ" heads the surface), in the surface and bulk respectively, then we will have:

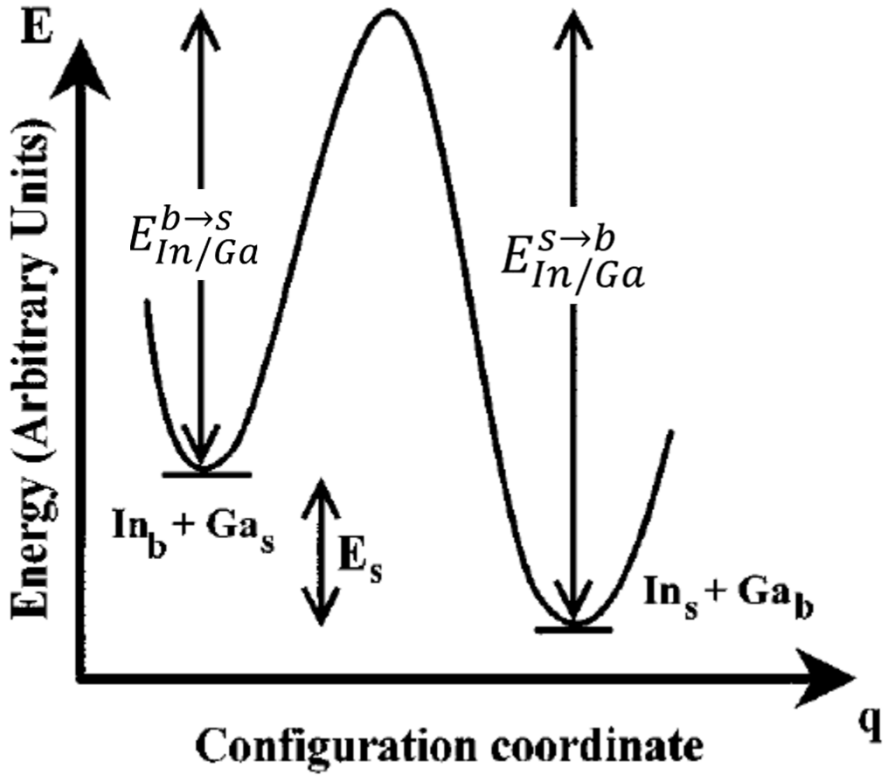
$$X^s(n-1) + X_\Phi = X^s(n) + X^b(n)$$



Segregation Energy

- $E_{In/Ga}^{b\rightarrow s}$ = Barrier energy for “In” atom segregation to the surface (free energy of the system).
- $E_{In/Ga}^{s\rightarrow b}$ =Barrier energy for “In” atom segregation to the bulk or “Ga” atom segregation to the surface.
- $E_s = E_{In/Ga}^{s\rightarrow b} - E_{In/Ga}^{b\rightarrow s}$

  ≡ Segregation Energy.



Segregation Energy

- In $A_xB_{1-x}C/BC$ system ("A" and "B" are group III and "C" is a group V element), segregation driving force, "E_s", is determined as:

$$E_s = E_{A/B}^{s\to b} - E_{A/B}^{b\to s}$$

- $E_{A/B}^{s\to b}$ انرژی هست که اگر اتم A از سطح بخواهد با اتم B از بالک جابجا شود.
- $E_{A/B}^{b\to s}$ انرژی هست که اگر اتم A از بالک بخواهد با اتم B از سطح جابجا شود.
- بنابر این اگر $E_{A/B}^{s\to b}$ بزرگتر از $E_{A/B}^{b\to s}$ باشد این به معنی انست که اتم A از سطح به بالک نمی رود زیرا انرژی زیادتری می خواهد نسبت به آمدن به سطح، بنابر این مهاجرت به سطح برای A اتفاق می افتد و "E_s" مثبت خواهد بود (انرژی مهاجرت برای اتم A مثبت است).

Exchange Rate

- Two exchange processes are competing during the growth:

1- Exchange between the atoms in the bulk with the atoms on the surface:

The exchange process is achieved by overcoming an energy barrier $E_{A/B}^{b\to s}$

with an exchange rate, "$P_{A/B}^{b\to s}$": $$P_{A/B}^{b\to s} = v_{A/B}^{b\to s} exp\left(-\frac{E_{A/B}^{b\to s}}{k_B T}\right)$$

- In which "*T*(K)" is growth temperature, "k_B" is Planck's constant, "$v_{A/B}^{b\to s}$" is atom "A" effective hopping frequency from the bulk to the surface.

2- Exchange between the atoms on the surface with the atoms in the bulk:

The reverse exchange is also possible; however, it needs to pass over the $E_{A/B}^{s\to b} = E_{A/B}^{b\to s} + Es$ energy barrier and has an reverse exchange rate, "$P_{A/B}^{s\to b}$":

$$P_{A/B}^{s\to b} = v_{A/B}^{s\to b} exp\left(-\frac{E_{A/B}^{s\to b}}{k_B T}\right)$$

Exchange Rate

- "$v_{A/B}^{b\to s}$" is the vibration frequency which is about $2 \times 10^{10} s^{-1}$ near the surface and $1.16 \times 10^{15} s^{-1}$ in the bulk (PRB_40_10449).
- "$v_{A/B}^{b\to s}$" and "$v_{A/B}^{s\to b}$" are combination of surface and bulk lattice vibration frequencies about 10^{13} s^{-1} for all III-V material (PRB_40_10449. PRB-64-81305; APL-66-52).

Dynamic of Atoms Concentration

- Assuming that the segregation is only due to the exchange processes, the balance of the incoming to and leaving atoms from the surface gives the evaluation of the number of atom “A” on the surface.
- Therefore, the evolution of the number of “A” surface atoms is given by the balance of incoming and leaving “A” atoms:

$$\frac{dX_A^s(t)}{dt} = \underbrace{\Phi_A + P_{A/B}^{b\to s} X_A^b(t) X_B^s(t)}_{\text{Incoming atoms to surface}} - \underbrace{P_{A/B}^{s\to b} X_A^s(t) X_B^b(t)}_{\text{Leaving atoms from surface}} \qquad \text{(Eq-12)}$$

- In which, “Φ_A” is the impinging flux of atom “A” in ML/s, $X^s_A(t)$ and $X^b_A(t)$ are the concentration of atom “A” at time “t” in fraction of ML on the surface or in the bulk, respectively.

Dynamic of Atoms Concentration

- جمله $P_{A/B}^{b\to s}X_A^b(t)X_B^s(t)$ بیان می کند که نرخ میزان آمدن اتمهای A از بالک به سطح بستگی دارد به Exchange Rate و میزان اتمهای A در بالک که به سطح می آیند (اگر در بالک هیچ اتم A نباشد پس چیزی به سطح نمی آید) و میزان اتمهای B سطح که به بالک می رود (اگر هیچ اتم B در سطح نباشد پس هیچ اتم A به سطح نمی آید).

- At high substrate temperature, "T", the exchange rates, "$P_{A/B}^{b\to s}$" and "$P_{A/B}^{s\to b}$", become sufficiently high to yield the flux term, "Φ_A", negligible with respect to the exchange terms in Eq-12.

Stationary Case

- Question: Let's assume atom "A" is segregating to the surface.
- When we have no incoming flux ($\Phi_A=\Phi_B=0$, this is equivalent to a very high growth temperature), if we wait long enough, all atom "A" from bulk segregate to the surface or there will be an equilibrium of incoming and outgoing atom "A" from surface?
- Answer: At stationary state of the system, we have:

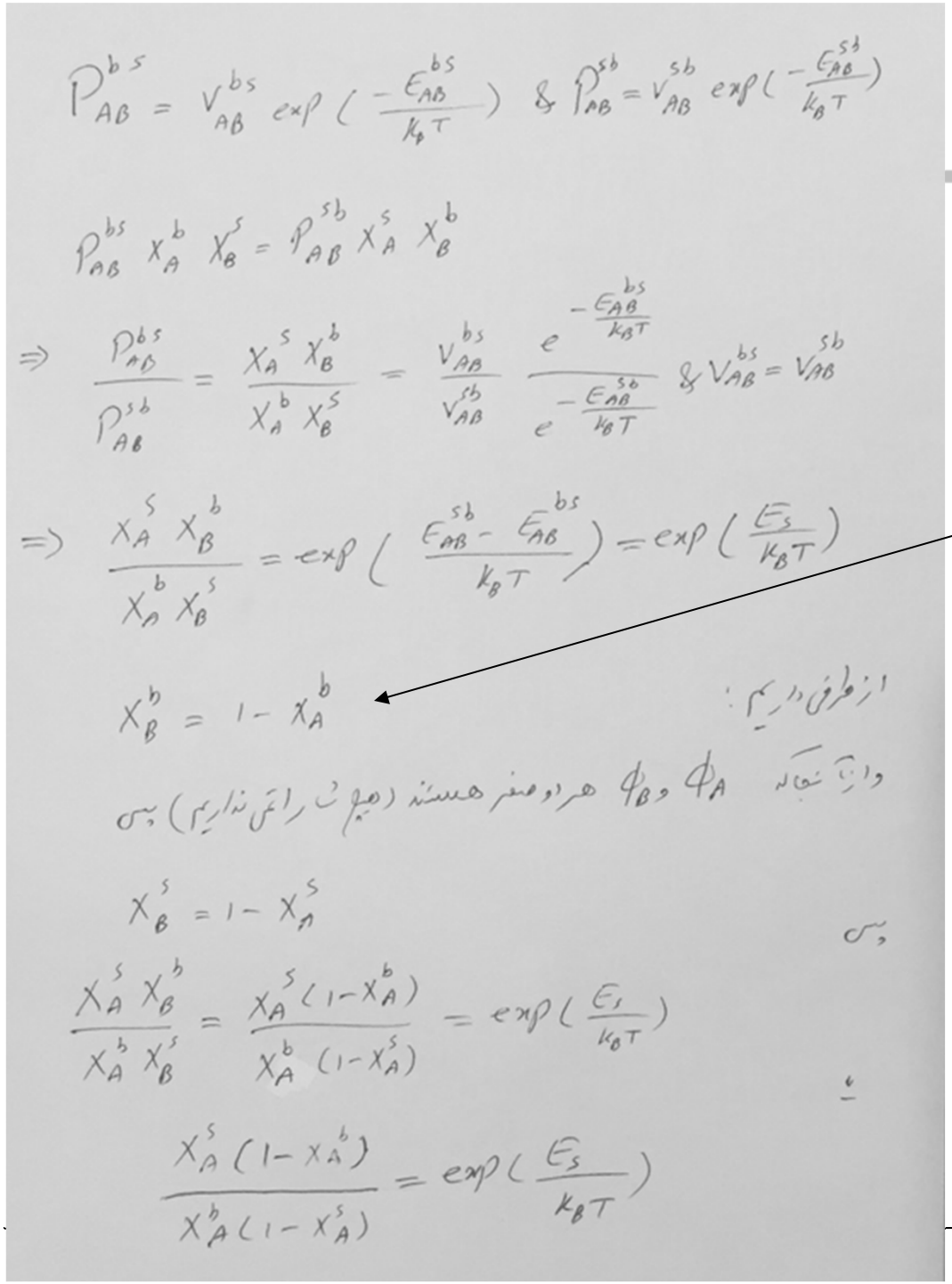
$$\frac{dX_A^S(t)}{dt} = 0$$

- Which yields:

$$P_{A/B}^{b\to s} X_A^b(t) X_B^s(t) = P_{A/B}^{s\to b} X_A^s(t) X_B^b(t) \Rightarrow \frac{X_A^s(t)[1-X_A^b(t)]}{X_A^b(t)[1-X_A^s(t)]} = exp\left(\frac{E_s}{k_B T}\right)$$

- Which means at a very high substrate temperature, the kinetic model is equivalent to the thermodynamical model.

Driving $\frac{X_A^s(t)[1-X_A^b(t)]}{X_A^b(t)[1-X_A^s(t)]} = exp\left(\frac{E_s}{k_BT}\right)$



- This equation is not valid for the surface composition.
- On surface, the total composition of group III can be higher than 100% (rich surface).

Atoms Concentration

- On the other hand, due to the mass conservation for atoms at any given time "t", we have:

Group III % of atoms in each ML is 1

$$X_A^b(t) + X_B^b(t) = 1 \quad \text{(Eq-13)}$$

Mass Conservation for atom "A" in bulk and surface

$$X_A^s(t) + X_A^b(t) = X_A^s(0) + X_A^b(0) + \Phi_A t \quad \text{(Eq-14)}$$

$$X_B^s(t) + X_B^b(t) = X_B^s(0) + X_B^b(0) + \Phi_B t \quad \text{(Eq-15)}$$

- Adding Eq-14 with Eq-15, we have:

$$X_A^s(t) + X_A^b(t) + X_B^s(t) + X_B^b(t) = X_A^s(0) + X_A^b(0) + \Phi_A t + X_B^s(0) + X_B^b(0) + \Phi_B t$$

$$X_A^s(t) + X_B^s(t) + \underbrace{X_A^b(t) + X_B^b(t)}_{1} = X_A^s(0) + X_B^s(0) + \underbrace{X_A^b(0) + X_B^b(0)}_{1} + (\Phi_A + \Phi_B)t$$

$$\Rightarrow \quad X_A^s(t) + X_B^s(t) = X_A^s(0) + X_B^s(0) + (\Phi_A + \Phi_B)t \quad \text{(Eq-16)}$$

Energy Constants

- Using equations 12 to 15, we are able to predict the atomic concentration profile for different growth conditions.
- Since the exchange process relates to only “In” and “Ga” atoms, the energy barrier “$E_{In/Ga}^{b\rightarrow s}$” must be of the order of In-As and Ga-As binding energies, about 1.4 eV and 1.59 eV (PRB_40_6149).
- For $Ga_{0.8}In_{0.2}As/GaAs$ system, the experimental value for “E_s“ is about 0.2 eV and “$E_{In/Ga}^{b\rightarrow s}$” is 1.8 eV for a substrate temperature T≥500ºC (PRB_40_6149; JVSTB_11_1413; APL_61_2096).
- The restriction for the temperature for this model comes from the fact that this model is valid as long as group III atom evaporation is negligible.

Segregation Simulation Equations

- For plotting segregation concentrations, we need to find: $X_B^s(t)$, $X_B^b(t)$, $X_A^s(t)$, and $X_A^b(t)$.
- From Eq-12 we have: $\frac{dX_B^s(t)}{dt} = \Phi_B + P_{A/B}^{b\to s} X_B^b(t) X_A^s(t) - P_{A/B}^{s\to b} X_B^s(t) X_A^b(t)$ (Eq-17)
- From Eq-15 we have: $X_B^b(t) = -X_B^s(t) + X_B^s(0) + X_B^b(0) + \Phi_B t$ (Eq-18)
- From Eq-16 we have: $X_A^s(t) = -X_B^s(t) + X_A^s(0) + X_B^s(0) + (\Phi_A + \Phi_B)t$ (Eq-19)
- From Eq-14 we have: $X_A^b(t) = -X_A^s(t) + X_A^s(0) + X_A^b(0) + \Phi_A t$ (Eq-20)
- Initial values for each concertation (at t=0) can be deduced from boundary condition (i.e. substrate surface where there was no deposition).

Double-atom Segregation Model

Segregation In $Al_yGa_{1-y}As/In_xGa_{1-x}As$

- In $\mathbf{Al_yGa_{1-y}As/In_xGa_{1-x}As}$ system, segregation takes place between three atoms: Al, Ga, and In.
- Therefore, unlike the case $Ga_xIn_{1-x}As/GaAs$, in which we used four equations to describe the segregation between Ga and In, we now have to derive a new set of six equations for $\mathbf{Al_yGa_{1-y}As/In_xGa_{1-x}As}$ system.
- Our approach is similar to the $Ga_xIn_{1-x}As/GaAs$ case, and we use the same laws and principles.
- From the conservation of mass law, at any given time, for each of Al, Ga, and In we have the following equations:

For In: $$X^s_{In}(t) + X^b_{In}(t) = \phi_{In}t + X^s_{In}(0) + X^b_{In}(0) \quad \text{(Eq-21)}$$

For Al: $$X^s_{Al}(t) + X^b_{Al}(t) = \phi_{Al}t + X^s_{Al}(0) + X^b_{Al}(0) \quad \text{(Eq-22)}$$

For Ga: $$X^s_{Ga}(t) + X^b_{Ga}(t) = \phi_{Ga}t + X^s_{Ga}(0) + X^b_{Ga}(0) \quad \text{(Eq-23)}$$

Segregation In $Al_yGa_{1-y}As/In_xGa_{1-x}As$

- The group III atoms share in the bulk is filled with Al, In, and Ga atoms at any given time; thus, we have:

$$X_{In}^{s} + X_{Ga}^{b} + X_{Al}^{b} = 1 \quad \text{(Eq-24)}$$

- Now, we have to derive two differential equations describing the rate of change in the concentration of atoms at the surface layer with time.
- For this purpose, we need to rewrite such equations for all three materials of Al, Ga, and In.
- For instance, if we choose Al and In, due to the conservation of mass law, the rate of change in the concentration of atoms at the surface layer equals the rate of atoms incoming this layer (X_{Al}^{in}) minus the rate of atoms leaving this layer (X_{Al}^{out}):

$$\frac{dX_{Al}^{s}}{dt} = X_{Al}^{in} - X_{Al}^{out} \quad \text{(Eq-25)}$$

Segregation In $Al_yGa_{1-y}As/In_xGa_{1-x}As$

- X_{Al}^{in} consists of two terms:

$$X_{Al}^{in} = \phi_{Al} + X_{Al}^{b\rightarrow s} \quad \text{(Eq-26)}$$

- ϕ_{Al} being the impinging flux of Al in ML/s, and $X_{Al}^{b\rightarrow s}$ being the rate of Al atoms segregating from the bulk to the surface layer.
- For calculation of $X_{Al}^{b\rightarrow s}$, we should consider the exchange between Al-Ga and Al-In.
- The rate, by which Al atoms segregate to the surface replacing Ga atoms, equals:

$$X_{Al/Ga}^{b\rightarrow s} = P_{Al/Ga}^{b\rightarrow s}\, X_{Al}^{b}\, X_{Ga}^{s} \quad \text{(Eq-27)}$$

- Where $P_{Al/Ga}^{b\rightarrow s}$ is the exchange rate:

$$P_{Al/Ga}^{b\rightarrow s} = v_{Al/Ga}^{b\rightarrow s} \exp\left(-\frac{E_{Al/Ga}^{b\rightarrow s}}{k_B T}\right) \quad \text{(Eq-28)}$$

Segregation In $Al_yGa_{1-y}As/In_xGa_{1-x}As$

- The rate, by which Al atoms segregate to the surface replacing “In” atoms, equals:

$$X_{Al/In}^{b\rightarrow s} = P_{Al/In}^{b\rightarrow s}\, X_{Al}^{b}\, X_{In}^{s} \qquad \text{(Eq-29)}$$

- Where $P_{Al/In}^{b\rightarrow s}$ is the exchange rate:

$$P_{Al/In}^{b\rightarrow s} = v_{Al/In}^{b\rightarrow s}\exp\left(-\frac{E_{Al/In}^{b\rightarrow s}}{k_B T}\right) \qquad \text{(Eq-30)}$$

- Therefore, for $X_{Al}^{b\rightarrow s}$ we have two terms:

$$X_{Al}^{b\rightarrow s} = P_{Al/Ga}^{b\rightarrow s}\, X_{Al}^{b}\, X_{Ga}^{s} + P_{Al/In}^{b\rightarrow s}\, X_{Al}^{b}\, X_{In}^{s} \qquad \text{(Eq-31)}$$

- And:

$$X_{Al}^{in} = \phi_{Al} + P_{Al/Ga}^{b\rightarrow s}\, X_{Al}^{b}\, X_{Ga}^{s} + P_{Al/In}^{b\rightarrow s}\, X_{Al}^{b}\, X_{In}^{s} \qquad \text{(Eq-32)}$$

Segregation In $Al_yGa_{1-y}As/In_xGa_{1-x}As$

- For X_{Al}^{out}, we need to calculate the rate of segregation of Al from the surface to the bulk.
- The rate, by which Al atoms segregate to the bulk replacing Ga atoms, are equal:

$$X_{Al/Ga}^{s\rightarrow b} = P_{Al/Ga}^{s\rightarrow b} X_{Al}^{s} X_{Ga}^{b} \quad \text{(Eq-33)}$$

- Where $P_{Al/Ga}^{s\rightarrow b}$ is the exchange rate:

$$P_{Al/Ga}^{s\rightarrow b} = v_{Al/Ga}^{s\rightarrow b} \exp\left(-\frac{E_{Al/Ga}^{s\rightarrow b}}{k_B T}\right) \quad \text{(Eq-34)}$$

- The rate, by which Al atoms segregate to the bulk replacing “In” atoms, are equal:

$$X_{Al/In}^{s\rightarrow b} = P_{Al/In}^{s\rightarrow b} X_{Al}^{s} X_{In}^{b} \quad \text{(Eq-35)}$$

Segregation In $Al_yGa_{1-y}As/In_xGa_{1-x}As$

- Where $P_{Al/In}^{s\rightarrow b}$ is the exchange rate:

$$P_{Al/In}^{s\rightarrow b} = v_{Al/In}^{s\rightarrow b}\exp\left(-\frac{E_{Al/In}^{s\rightarrow b}}{k_B T}\right) \quad \text{(Eq-36)}$$

- Therefore, for X_{Al}^{out} we have:

$$X_{Al}^{out} = P_{Al/Ga}^{s\rightarrow b} X_{Al}^{s} X_{Ga}^{b} + P_{Al/In}^{s\rightarrow b} X_{Al}^{s} X_{In}^{b} \quad \text{(Eq-37)}$$

- Thus, the rate of change in the concentration of Al atoms at the surface layer equals:

$$\frac{dX_{Al}^{s}}{dt} = X_{Al}^{in} - X_{Al}^{out} = \phi_{Al} + P_{Al/Ga}^{b\rightarrow s} X_{Al}^{b} X_{Ga}^{s} + P_{Al/In}^{b\rightarrow s} X_{Al}^{b} X_{In}^{s} - P_{Al/Ga}^{s\rightarrow b} X_{Al}^{s} X_{Ga}^{b} - P_{Al/In}^{s\rightarrow b} X_{Al}^{s} X_{In}^{b} \quad \text{(Eq-38)}$$

Segregation In $Al_yGa_{1-y}As/In_xGa_{1-x}As$

- Similarly, for Ga atoms, we obtain:

$$\frac{dX_{Ga}^{s}}{dt} = X_{Ga}^{in} - X_{Ga}^{out} = \phi_{Ga} + P_{Ga/Al}^{b\rightarrow s}\, X_{Ga}^{b}\, X_{Al}^{s} + P_{Ga/In}^{b\rightarrow s}\, X_{Ga}^{b}\, X_{In}^{s} - P_{Ga/Al}^{s\rightarrow b}\, X_{Ga}^{s}\, X_{Al}^{b} - P_{Ga/In}^{s\rightarrow b}\, X_{Ga}^{s}\, X_{In}^{b} \quad \text{(Eq-39)}$$

- Therefore, we will have the following set of six equations:

$$X_{In}^{s} + X_{In}^{b} = \phi_{In}t + X_{In}^{s}(0) + X_{In}^{b}(0) \quad \text{(Eq-40)}$$

$$X_{Al}^{s} + X_{Al}^{b} = \phi_{Al}t + X_{Al}^{s}(0) + X_{Al}^{b}(0) \quad \text{(Eq-41)}$$

$$X_{Ga}^{s} + X_{Ga}^{b} = \phi_{Ga}t + X_{Ga}^{s}(0) + X_{Ga}^{b}(0) \quad \text{(Eq-42)}$$

$$X_{In}^{s} + X_{Ga}^{b} + X_{Al}^{b} = 1 \quad \text{(Eq-43)}$$

Segregation In $Al_yGa_{1-y}As/In_xGa_{1-x}As$

$$\frac{dX_{Al}^{s}}{dt} = X_{Al}^{in} - X_{Al}^{out} = \phi_{Al} + P_{Al/Ga}^{b\rightarrow s}\ X_{Al}^{b}\ X_{Ga}^{s} + P_{Al/In}^{b\rightarrow s}\ X_{Al}^{b}\ X_{In}^{s} - P_{Al/Ga}^{s\rightarrow b}\ X_{Al}^{s}\ X_{Ga}^{b} - P_{Al/In}^{s\rightarrow b}\ X_{Al}^{s}\ X_{In}^{b} \quad \text{(Eq-44)}$$

$$\frac{dX_{Ga}^{s}}{dt} = X_{Ga}^{in} - X_{Ga}^{out} = \phi_{Ga} + P_{Ga/Al}^{b\rightarrow s}\ X_{Ga}^{b}\ X_{Al}^{s} + P_{Ga/In}^{b\rightarrow s}\ X_{Ga}^{b}\ X_{In}^{s} - P_{Ga/Al}^{s\rightarrow b}\ X_{Ga}^{s}\ X_{Al}^{b} - P_{Ga/In}^{s\rightarrow b}\ X_{Ga}^{s}\ X_{In}^{b} \quad \text{(Eq-45)}$$

Kinetic Model Examples

Kinetic Model of In Segregation

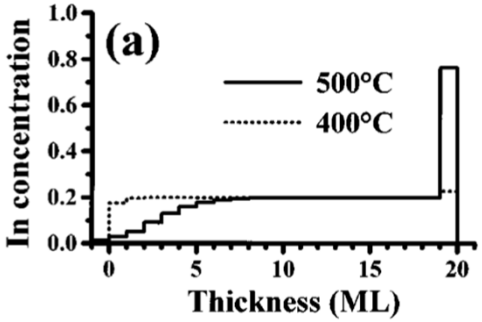
System: InAs/GaAs

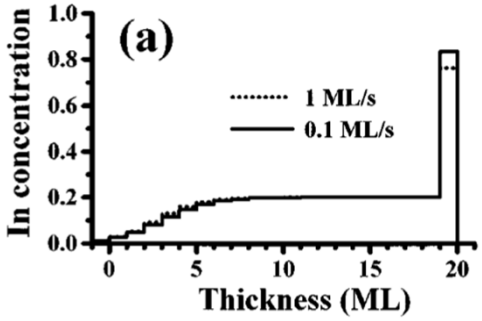
$E_{In/Ga}^{b\rightarrow s} = 1.8\ ev$

$E_{In/Ga}^{s\rightarrow b} = 2\ ev$

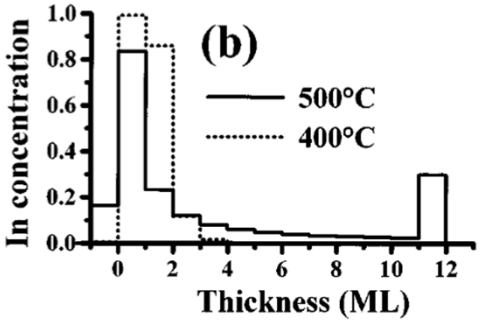
$E_s = 0.2\ ev$

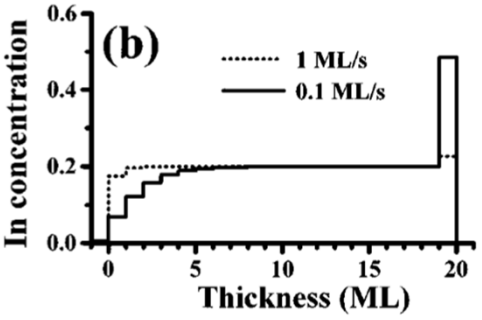
a: 20ML $In_{0.2}\ Ga_{0.8}As/GaAs$



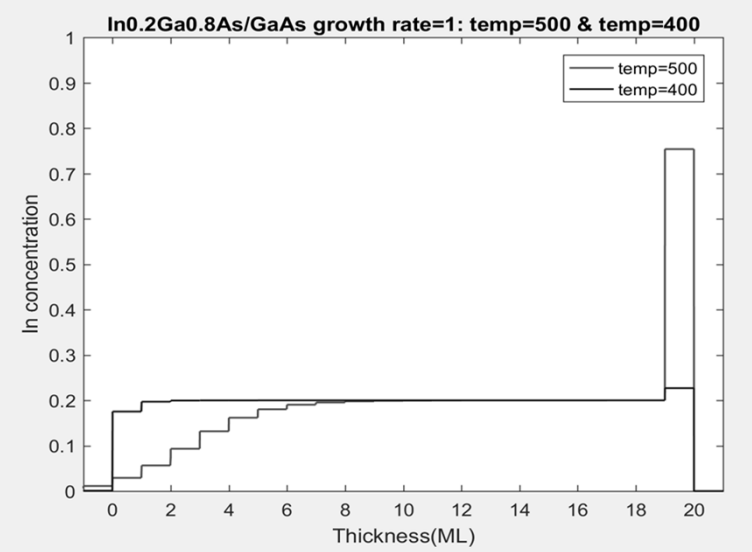


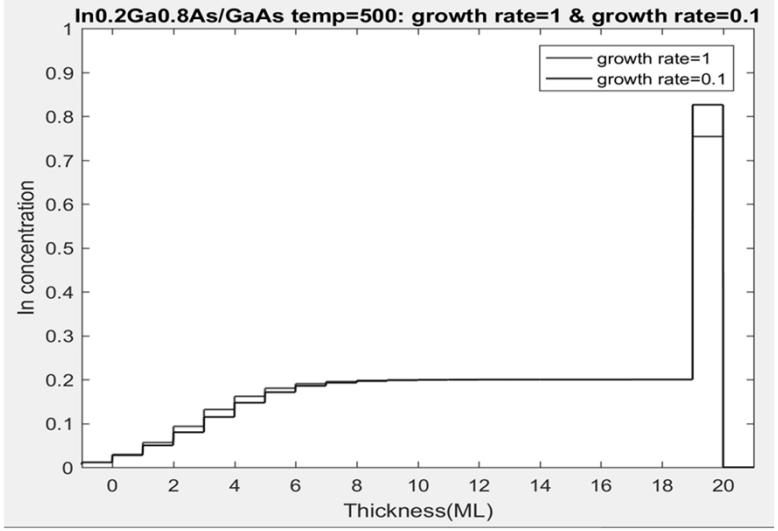
b:10ML GaAs/2ML InAs/GaAs

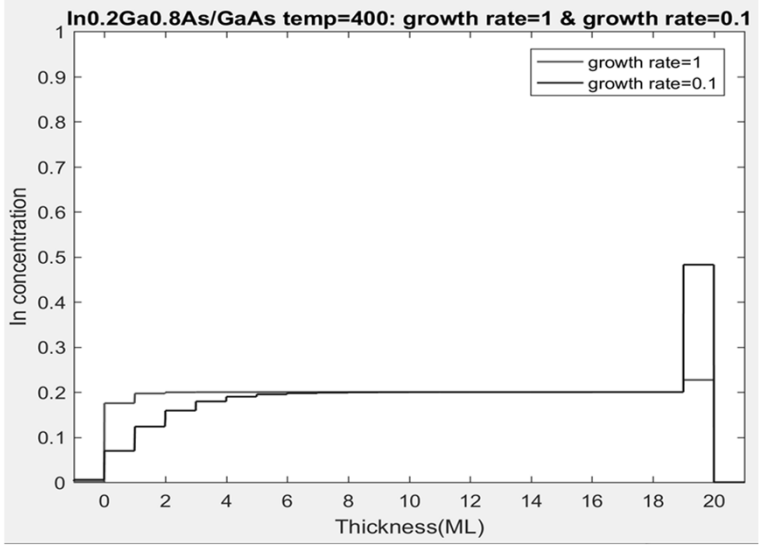


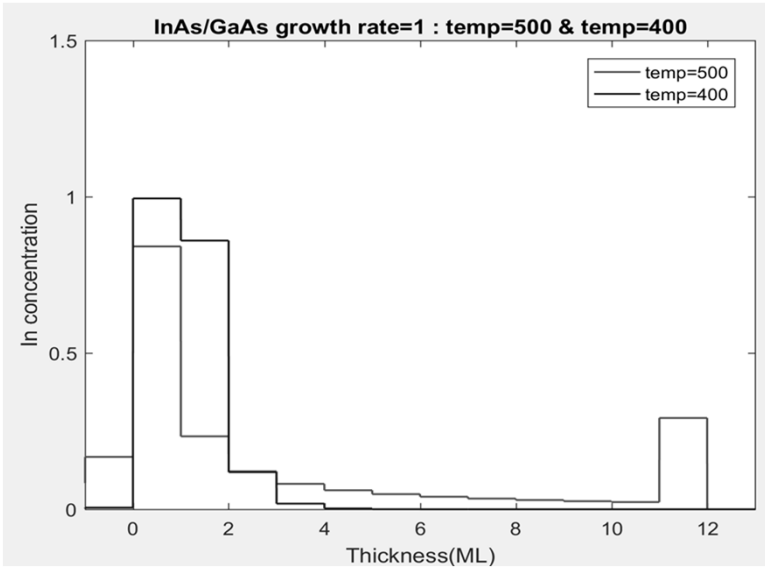


شبیه سازی مدل جنبشی توسط آقای مهندس مختاری









Kinetic Model of Ga Segregation

System: AlAs/GaAs

$E_{Ga/Al}^{b\rightarrow s}$ = 1.7 ev

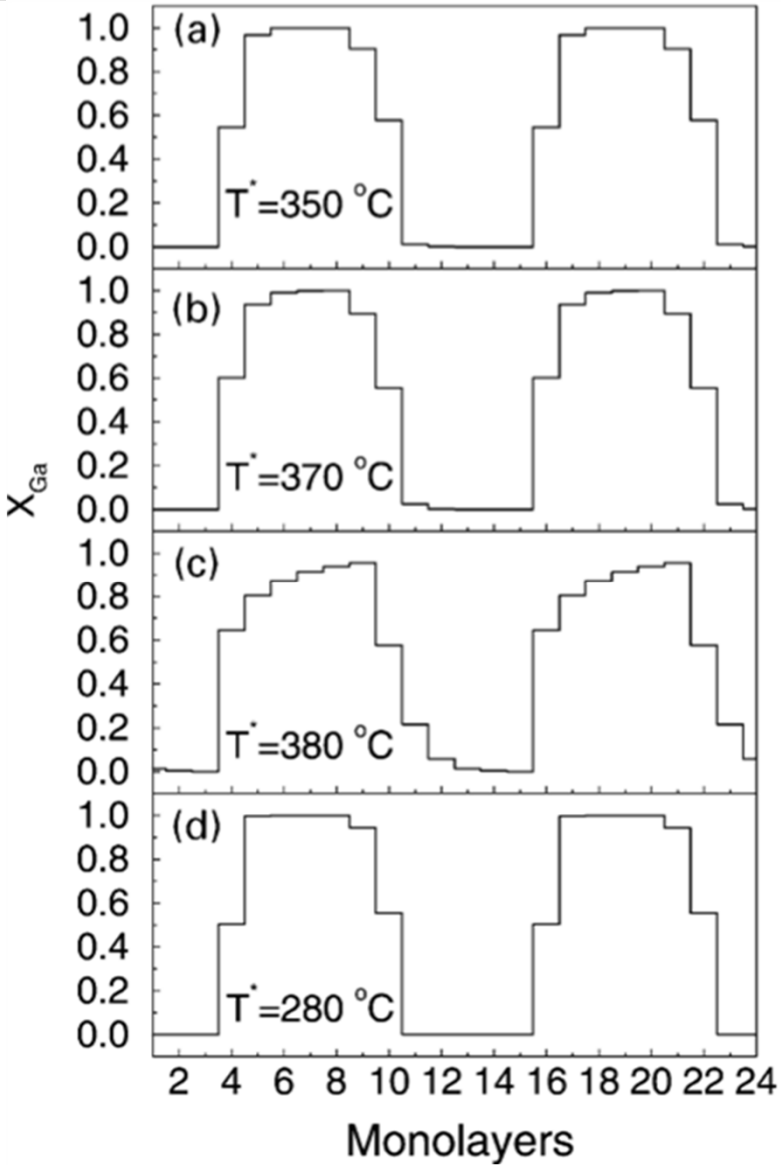
$E_{Ga/Al}^{s\rightarrow b}$ = 1.8 ev

E_s = 0.1 ev

6ML GaAs/6ML AlAs/GaAs

sample	T_{growth} (℃)	V_{growth} (ML/s)	P_{As} (mbar)	t_{int} (s)	T^* (℃)
a	570	0.5	2×10^{-7}	30	350
b	570	0.5	1×10^{-7}	30	370
c	580	0.5	1.1×10^{-7}	15	380
d	485	0.5	1.1×10^{-7}	120	280

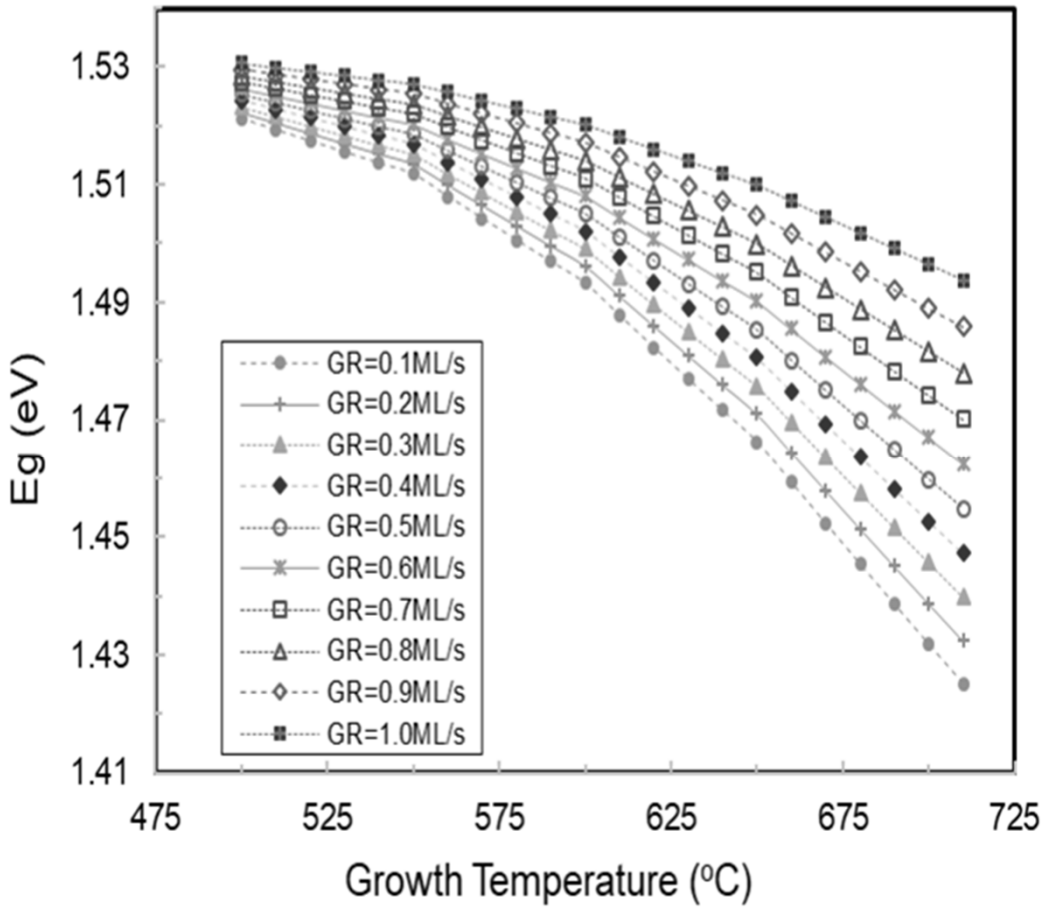
- T^* دمای موثر که در معادلات قرار می دهیم.
- t_{int} زمان استراحت پس از رشد کامل یک لایه.



دمای رشد و گاف انرژی در $Al_{0.35}Ga_{0.65}As/GaAs$

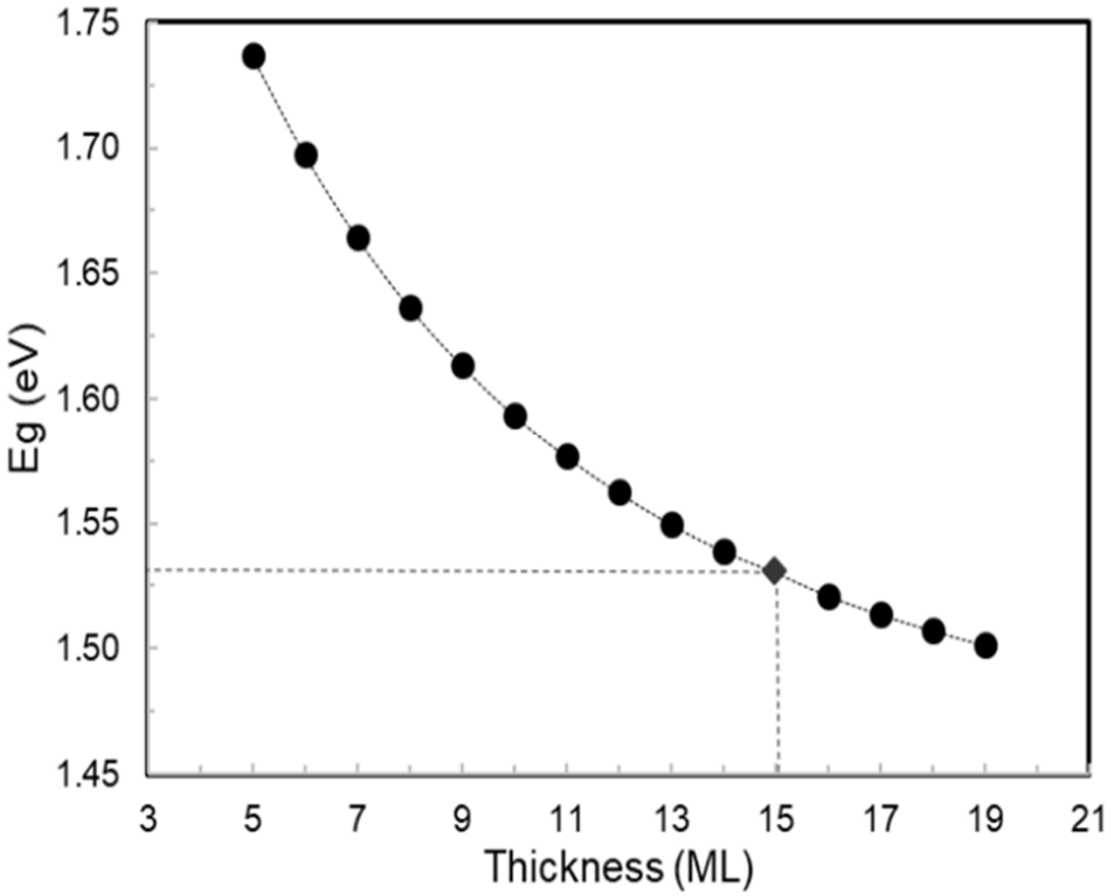
- عدم تقارن ترکیب در رابط ها منجر به تغییر تراز باند انرژی ساختارهای کوانتومی می شود که باعث تغییر در خواص نوری می شود.
- بنابراین ، برای طراحی یک دستگاه اپتوالکترونیکی بر اساس ساختارهای نیمه هادی III-V، پیش بینی و جبران تغییر مشخصات غلظت به دلیل مهاجرت اتم ها حائز اهمیت است.
- شکل بعد وابستگی به دما و سرعت رشد از $Al_{0.35}Ga_{0.65}As/GaAs$ پهنای باند انرژی محاسبه شده به دلیل مهاجرت Gaرا نشان می دهد.
- از آن ، می توان دریافت که افزایش دمای رشد در نرخ رشد بالا 1ML/s از 500 تا 710 درجه سانتیگراد به تغییر 0.04eV> منجر میشود.در حالیکه با نرخ رشد کم 0.1ML/s باعث تغییر مجدد بیشتر در حدود 0.1eV می شود.
- این امر به این دلیل است که ، هنگامی که درجه حرارت رشد افزایش یافت، انرژی جداسازی گالیم نیز افزایش یافت. بنابراین، سرعت تفکیک افزایش یافته و پهنای باند انرژی سیستم کاهش یافته است.

دمای رشد و گاف انرژی در $Al_{0.35}Ga_{0.65}As/GaAs$



وابستگی به دما و سرعت رشد $Al_{0.35}Ga_{0.65}As$ / GaAs به دلیل تفکیک گالیم ، پهنای باند انرژی را محاسبه کرد.

دمای رشد و گاف انرژی در $Al_{0.35}Ga_{0.65}As/GaAs$



تغییرات شکاف باند انرژی محاسبه شده $Al_{0.35}Ga_{0.65}As$ / GaAs با در نظر گرفتن تفکیک Ga، برای ضخامت های مختلف GaAs در دمای رشد 710 درجه سانتیگراد و سرعت رشد 1ML/s محاسبه کرد.

- از شکل مقابل دیده می شود که با کاهش 4ML ضخامت چاه کوانتومی GaAs به 15ML، می توان به شکاف باند 1.53eV برای طول موج حدود 808 نانومتر دست یافت، که نزدیک به نتایج تجربی گزارش شده در سیستم های مشابه است.

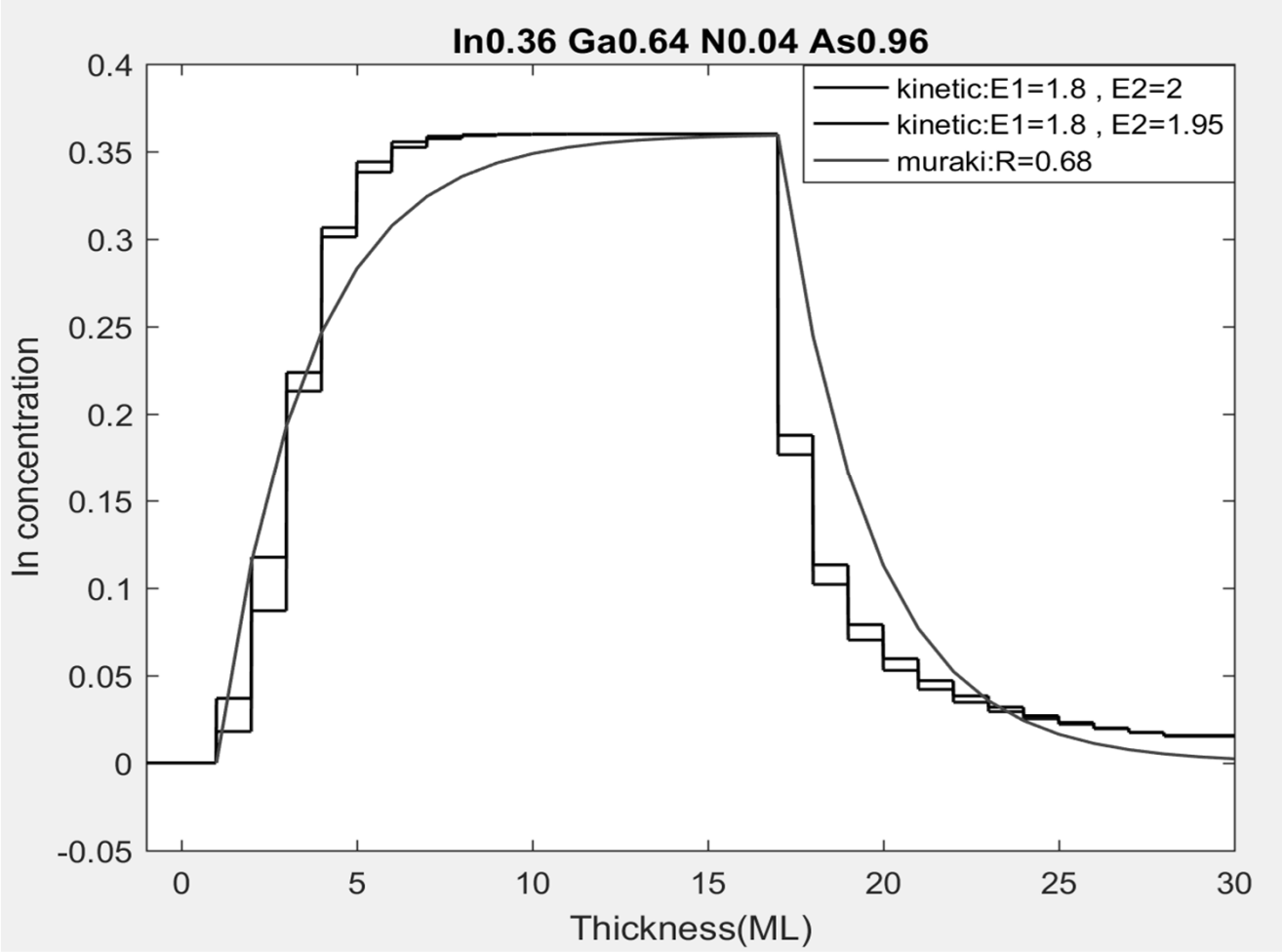
III-V Kinetic Model Segregation Constants

Semiconductors	E1 (eV)	E2 (eV)	Es (eV)	v_i (s^{-1})	Article
In→Ga	1.8	2	0.2	10^{13}	Dehease(APL_66_52)
Ga →Al	1.7	1.8	0.1	10^{13}	Zanelato(PE_10_587)
In→Al	1.79	2.08	0.29	10^{13}	Dorin(JAP_91_237)
Sb→As	1.68	1.75	0.07	10^{13}	Magri(PRB_64_81305)

یافتن ثوابت مدل جنبشی از روز منحنی های مدل Muraki

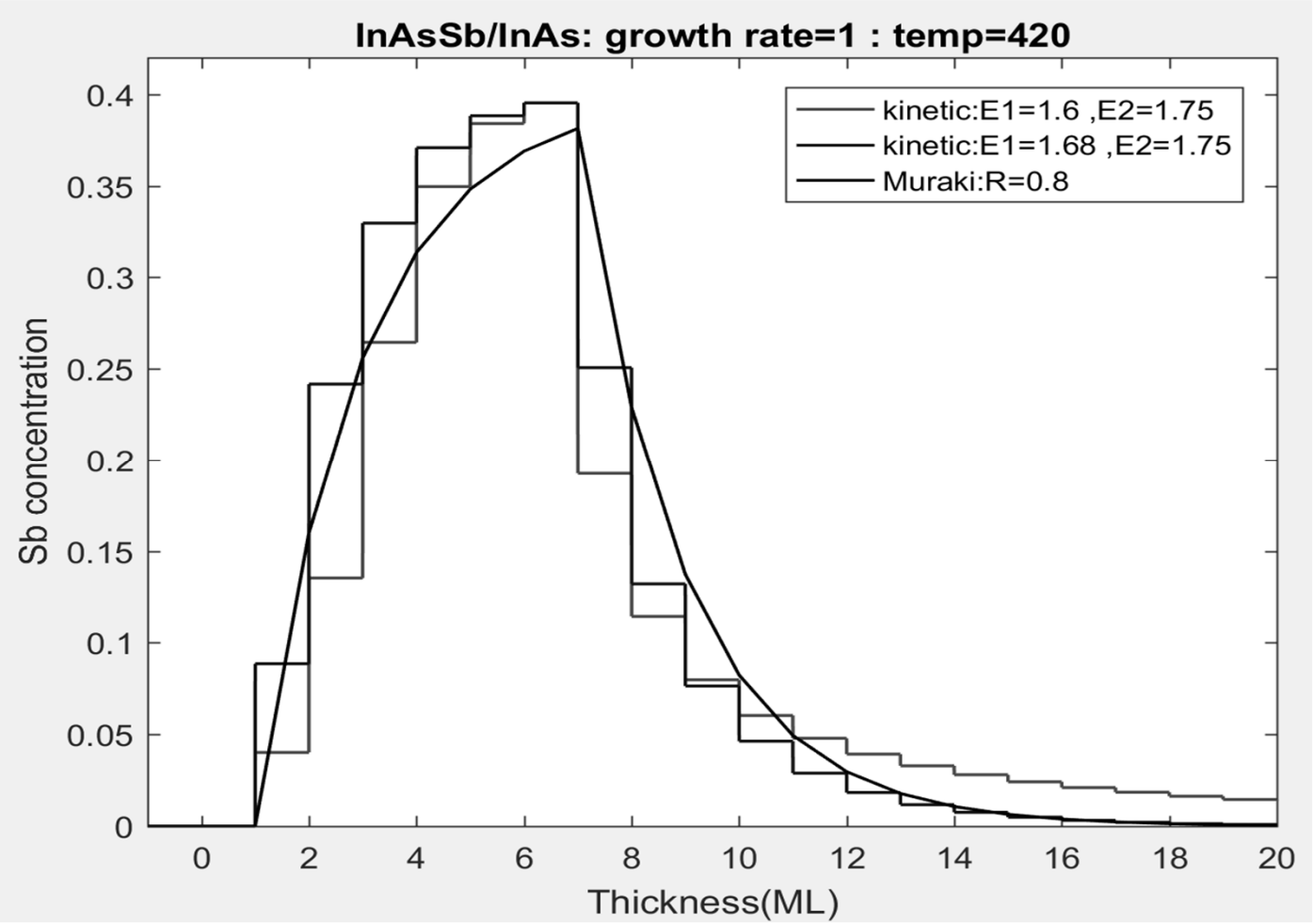
تطبیق دو مدل موراکی و جنبشی

$16ML In_{0.36}Ga_{0.64}N_{0.04}As_{0.96}/GaAs$



تطبیق دو مدل موراکی و جنبشی

6ML In $As_{0.6}Sb_{0.4}$/ 11 ML InAs



Comparing Different Models

مدل ها	نحوه اندازه گیری پارامتر ها	مزایا	معایب
Muraki	• پروفایل SIMS • تطبیق	• معادلات آسان • بیشترین تعداد مقاله و داده در بین دیگر مدل ها	• دقت پایین • تغییر پارامتر ها با تغییر شرایط رشد • مدل تجربی
Kinetic	تطبیق	• مدل علمی • دقت خوب • پارامترها با تغییر شرایط رشد تغییر نمی کنند	• معادلات پیچیده • دقت متوسط • داده های کم
Sigmoidal	تطبیق	• دقت عالی • مدل جدید و امکان کارهای متعدد بر روی آن	• تغییر پارامتر ها با تغییر شرایط رشد • مدل تجربی

Fluid Three-layer Exchange Model

Fluid Three-layer Exchange (F3LE)

- مدل تبادل سیال سه لایه (F3LE) که توسط Godbey و Ancona ارائه شده است میتواند توصیف بهتری از مهاجرت اتمها باشد.
- این مدل اولین بار برای یک سیستم ماده که در آن مهاجرت هر دو In و Sb اتفاق می افتد گزارش شده است.
- به خلاف دیگر مدل ها که در آن ها تبادل فقط بین دو لایه در نظر گرفته میشد،در مدل F3LE تبادل بین بالاترین سه لایه موجود اتفاق می افتد و یک نرخ انتشار سطحی نامحدود فرض میشود.
- وقتی که رشد لایه های جدید شروع میشود، تبادل اتمها بین بالاترین لایه(s) و دومین بالاترین لایه (s-1) و بین دومین بالاترین لایه (s-1)و سومین بالاترین لایه (s-2) اتفاق می افتد.
- زمانیکه لایه s به طور کامل رشد یافت، لایه s-2 دیگر در مکانیزم تبادل شرکت نمیکند و یک لایه جدید شروع به رشد کردن میکند که در نتیجه رشد و تبادل به طور همزمان اتفاق می افتند.
- این مدل از اصول و فرمول بندی مدل جنبشی استفاده می کند.

F3LE Formalism

- The composition of the 3 topmost layers taking part in the exchange is given as:

$$X_{In}^{s} + X_{Ga}^{s} = \frac{t}{\tau}$$

$$X_{In}^{s-1} + X_{Ga}^{s-1} = 1$$

$$X_{In}^{s-2} + X_{Ga}^{s-2} = 1$$

- In which, X_{In}^{s} denotes the concentration of “In” in the topmost layer, “t” is the time and “τ” is the time needed to complete the growth of one monolayer.

F3LE Formalism

- The composition of “In” in all 3 layers underlie mass balance equations:

$$\frac{dX_{In}^{s}}{dt} = \Phi_{In} + E_{s,s-1}$$

$$\frac{dX_{In}^{s-1}}{dt} = E_{s-1,s} + E_{s-1,s-2}$$

$$\frac{dX_{In}^{s-2}}{dt} = E_{s-2,s-1}$$

- In which $\Phi_{In} = \frac{x}{\tau}$ is the “In” incorporation rate and $E_{i,j}$ describes the exchange process as:

$$E_{i,i-1} = P_1 X_{Ga}^{i} X_{In}^{i-1} - P_2 X_{Ga}^{i-1} X_{In}^{i}$$

F3LE Formalism

- The time to grow one monolayer, τ, is determined from the growth time for the QWs which is 11 s in case of the GaInAs QW and 13 s in case of the GaAsSb QWs and the number of layers as determined by Muraki's model.
- With exchange probabilities P_1 and P_2 that are described as:

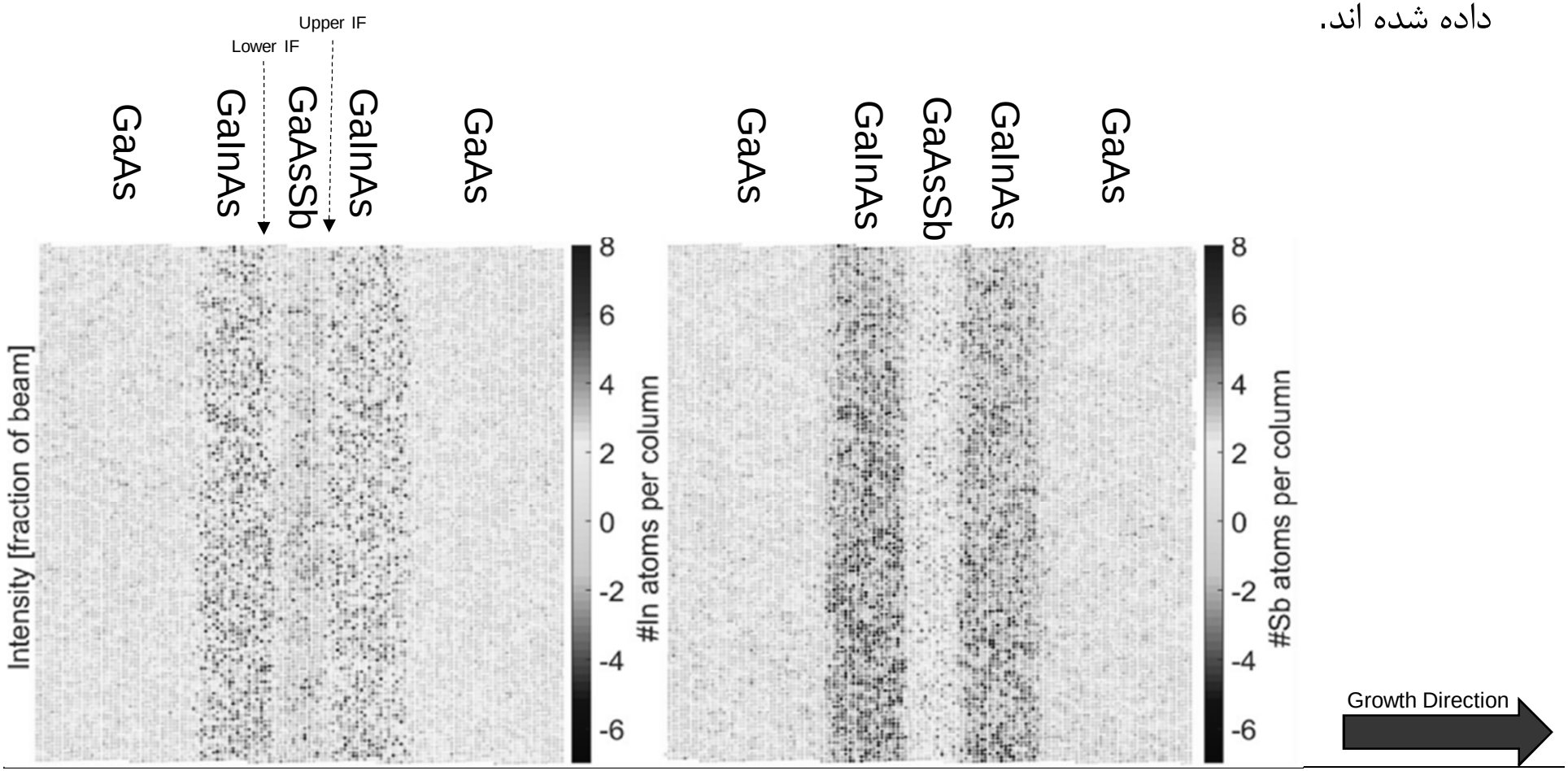
$$P_1 = v_1 e^{-\frac{E_1}{k_b T}} \quad \& \quad P_2 = v_2 e^{-\frac{E_2}{k_b T}}$$

- E_1 and E_2 are surface and bulk energies, while v_1 and v_2 are vibrational frequencies that describe a combination of surface and bulk lattice vibration and are normally chosen as $10^{13} s^{-1}$.
- "T" is the temperature and "k_b" is the Boltzmann constant.

Supporting Slides

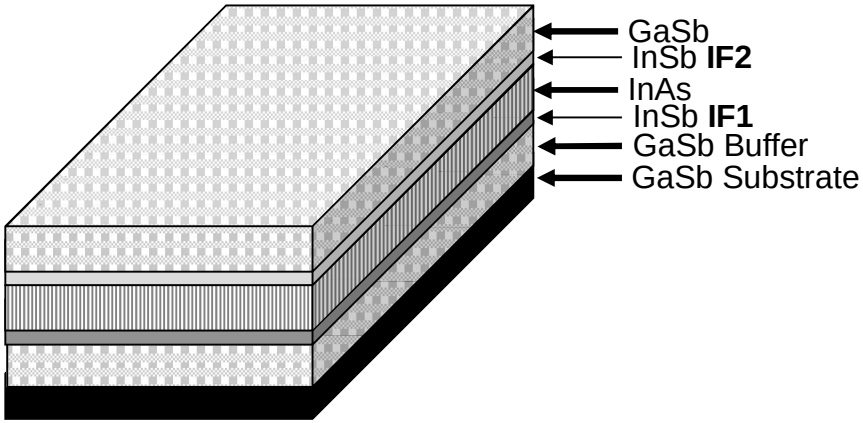
Muraki and F3LE Model

- در این مطالعه هر دو مدل موراکی و F3LE برای توصیف پروفایل تمرکز QW های مختلف به کار میروند.
- نقشه ترکیب بندی(Composition Map) (GaIn)As-QW و Ga(AsSb)-QWدر شکل زیر نشان داده شده اند.



Sb **Segregation in Type II SLS**

Non-Segregated



GaSb

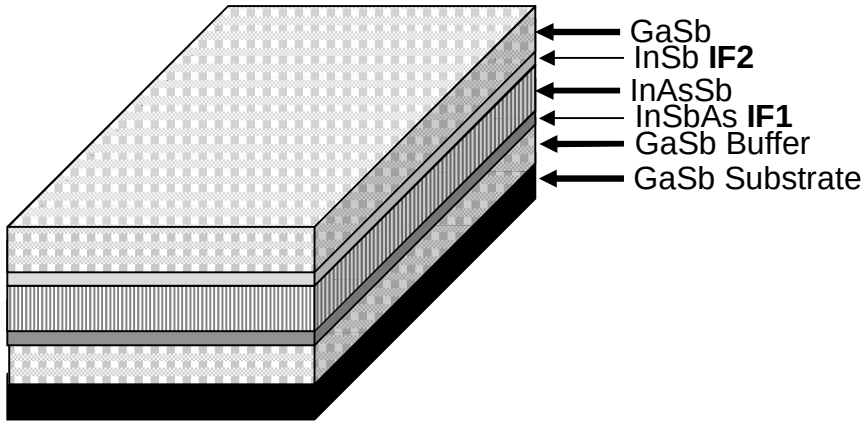
InSb -IF2

InAs

InSb -IF1

GaSb

Sb-Segregated



GaSb

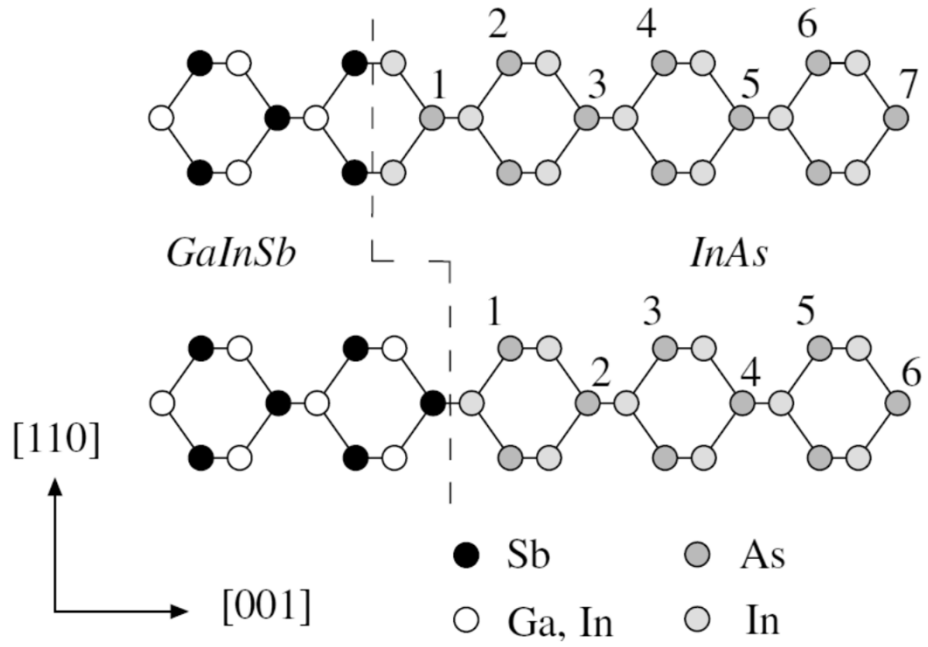
InSb -IF2

InAs (Sb Segregated InAs Layer)

InAsSb (Segregated Interface)-IF1

GaSb

Sb **Segregation Can Affect The Individual SLS Layer Thicknesses**



- Segregation can add to one layer and/or subtract from another one.
- It can cause adding to GaInSb layer.
- It can cause shifting one mono layer of InAs to the InGaSb layer.
- It can affect the interface composition. The interface can be either InSb or GaAs. It can.

- (001) Is a polar surface that has A or B.

Supporting Slides

Exercise

- In-As bond is stronger than In-Sb bond.
- Compare bond strength and length in:
    1. AlN, GaN, InN,
    2. AlP, GaP, InP
    3. AlAs, GaAs, InAs,
    4. GaSb, InSb, AlSb,
- Plot the results