Numerical study of atomic diffusion processes of copper on silver (110) surface: Cu/Ag (110)

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The aim of this paper is to study the diffusion of Cu adatom on Ag (110) by using the molecular dynamics simulation in the framework of the embedded atom method (EAM) as model of atomic interaction. Our simulation results predict that several diffusion processes such as simple jump, long jump and exchange mechanism may occur in the same system. The static barrier is calculated for each process by the drag method. The dynamic activation energy calculated from the Arrhenius law is in a good agreement with the static barrier. The presence of double jump is studied using velocity correlation function showing small contributions in diffusion process. Implications of these findings are discussed in more details.

1. Introduction

Understanding surface diffusion has been the goal of many investigations because of potential application in several areas. The diffusion of monomer on metal surface plays a crucial role in diverse areas as thin film and crystal growth [1-12]. It is one of the fundamental processes in surface science [13-16]. Many different diffusion mechanisms have been discovered. In fact, the diffusion of adatoms on metal surfaces may occur not only by uncorrelated hops between nearest-neighbor (NN) sites on the surface lattice, but also by exchanges (Ex) or by long jumps (in the following *jn* will indicate an *n*-sites jump).

The occurrence of long jumps (so-called *correlated jumps*) has been observed experimentally in different heterogeneous systems [17-21] such as Ir/W(110), Na/Cu(110),Pt/W(211) and Fe/W(110). Many experiment tools have been used for direct observation of surface diffusion processes such as Field-Ion Microscopy (FIM). This technique has led to the discovery of many novel atomic scale diffusion mechanisms [22,23] and it has been applied to study the diffusion on W(211) [17-20]. In diffusion of Re and Mo adatom on W(211) there was no evidence of long jump near room temperature. But for *Ir* and Rh adatoms on W(211), few long jumps were found(≈3%), and in the case of Pd/W(211) there was a significant fraction of correlated jumps (≈20%). Another experiment tool is the Scanning Tunnelling Microscopy (STM) [24] which can be used to manipulate atoms and moved them from one position to another [25-27]. Using STM, Linderoth et al. [20] found that not only simple jumps follow an Arrhenius law but also long jumps as in Pt/Pt(110) where the activation barrier for diffusion

(E_{d2}=0.89eV) is slightly larger than that for single jumps (E_{d1}=0.81eV). The presence of exchange mechanism was observed in many different systems [22]. The adatom cross-channel diffusion was experimentally discovered in W/Ir(110) [30] and predicted by molecular dynamics in Pt/Pt(110) and Ir/Pt(110) [31]. In more compact surface and by using molecular dynamics, the Cu [32] and others metals [33] shown that complicated exchange process occurs at high temperatures due to the correlation between all mechanism processes such simple jump-exchange or long jump-exchange.

The molecular dynamics (MD) simulation shows that in Ag/Ag(110) the simple jumps represent more than 90% of total number of jump at any temperature [34]. This percentage is in good agreement with the MD result of adatom diffusion along the straight steps on Ag(111) surface [35]. Therefore, the mobility of Ag corresponds to diffusion coefficient in the range of 10^{-6}-10^{-5} cm^{2}s^{-1}. At high temperature, both of helium scattering experiments [36] and embedded atom simulation [37] demonstrate that a strong anharmonicity appears in the surface phonons on Ag(110). The mean square vibrational amplitude of top-layer atoms increases strongly at high temperature that explains why the diffusion mechanism is complicated at high temperature in Ag(110) . In Cu/Cu(110) the long jumps are frequent and present 6-15% in total jump for wide range of temperature [38]. Studies using modified analytical embedded atom method (MAEAM) have shown that the Cu adatom on Cu(110) presents many different mechanism processes [39] and correlation between them.

In the present paper we study the diffusion of copper on Ag(110), availability of Arrhenius and the activation

barrier for each process. The contribution of long jump is examined by analyzing the velocity correlation function.

This paper is organized as follows. The Section.2 contains the model and the methods of calculations adopted in this work. In section 3 we present our findings about the diffusion of copper adatom on Ag (110) surface. We also calculate the static barrier by the drag method. In section 4 we present our conclusions.

2. Model and details of the calculations

In order to study the diffusion of adatom by using molecular dynamics method an adequate interaction potential was adopted. Several attempts have been made considering various models of interaction energy such as the pairwise potential as Lennard-Jones's or Morse's work [40,41].These kinds of potentials are usefully used to treat inert impurities such as He in metal, but are not applicable to chemically active impurities. Empirical potentials have also been made by introducing a many-body cohesive term in addition to the pairwise potential such as effective medium theory [42], glue model [43], many-body potentials developed by Rosato-Guillope-Legrand (RGL) [34,44] on the basis of the second-moment approximation to the tight binding model [45] and Embedded Atom Method (EAM) [46].

To follow the adatom trajectories, the interaction potential adopted in this work is the EAM. This method which is widely used in this context consists of semi empirical method based on approximation of local density of functional theory.

$$E = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} V_{ij}(r_{ij}) + \sum_i F_i(\rho_{h,i}) \qquad (1)$$

where ρ_h is the electron density of the unperturbed host, V_{ij} is the pair potential and r_{ij} is the distance between atom i and atom j. The second term describes the atom environment. To find the rate of atomic jumps, one has to study the diffusional dynamics, either by the MD simulation, or with the help of a more simple approach. The rate jump σ_j is obtained at each temperature. It is calculated by dividing the total number of jumps by the simulation time. On the other hand, according to the usual phenomenological Arrhenius law, the rate jump is given by

$$\sigma_j = \sigma_j^0 \exp\left(-\frac{E_D}{k_B T}\right) \qquad (2)$$

More generally, the activation barrier E_D for the different diffusion processes depends both on the direction of the move and on the numbers of neighbors of the moving adatom. In the present work the prefactor σ_j^0 and E_D are both assumed as T-independent. Indeed, theoretical calculation on Ag [47,48], Cu [34,43,49-51] and Ni [34] self-diffusion on the (100) surface assumes that the activation barrier for jump diffusion should decrease with temperature in the framework of transition state theory and the quasiharmonic approximation to the lattice dynamics. The calculations made by Kürpick [52] show that when the activation barriers decrease the prefactors decrease in

the same time. The single-particle diffusion coefficient D is an important physical quantity, since it is related to adatom mean square displacement through the Einstein relation:

$$D = \lim_{t \to \infty} \frac{\langle |R(t) - R(0)|^2 \rangle}{2dt} \qquad (3)$$

Where d denote the Euclidian dimension, and R(t) is the position vector of the particle at time t. In a jump-theory [Ref.38] framework the coefficient of diffusion is given by

$$D = \frac{1}{2} a \sigma_j \sum_l l^2 p_l \qquad (4)$$

Where a is the distance between adjacent sites and p_l is the probability to have an l-sites jump.

3. Results and discussions

Our simulation box consists of 6 layers, where each layer contains 120 atoms. The atoms of (110) surface are lined up to forming channel called the channel of diffusion (Fig.1). The channel geometry suggests that the adatom diffusion may be occurs by jump process.

Table 1. This table summarizes the Static potential barrier data.

Jump Process						
System	EAM	EA (AFW)	EA (VC)	RGL	EM	CEM, MD-MC/CEM
Ag/Ag	0.31(f)	0.32 (a)	0.25 (a)	0.28 (b)	0.29 (d)	0.26 ,0.25 (c)
Cu/Cu	0.23(f)	0.24(a)	0.53 (a)	0.23 (b)	0.29 (d), 0.18(e)	0.08,0.26 (c)
Ag/Cu	0.24(f)					
Cu/Ag	0.27					

a-   From Liu et al (Ref. [54])
b-   From Montalenti and Ferrando (Ref. [38])
c-   From Perkins and DePriste (Ref. [55])
d-   From Slotz et al. (Ref. [56])
e-   From Hansan et al. (Ref. [57])
f-   From Sbiaai et al. (Ref. [58])

The total simulation time is 30 ns and we study the adatom diffusion at different temperatures from 300K to 400K. The periodic boundary conditions are applied in the plane surface (*x* and *y* direction). When the simulation box is constructed, we take into account the dilatation of the system caused by the temperature. Far from the fusion temperature, the dilatation follows a linear regime [36] (Eq.5).

$$a_{cell} = a_{cell}(T_0)(1 - \alpha(T - T_0)) \qquad (5)$$

a_{cell} is the cell parameter, T_0 is the initial temperature (generally $T_0 = 0 K$), and α is the factor of dilatation [53] which depends on the properties of the system under consideration.

3.1 In- Channel mobility

The jump processes (simple and long jumps) are considered in this part. The time of simulation is the time when the first exchange occurs. The atoms evolution in time and space is determined by the numerical solution of the classical equation of motion including the potential of Eq.1.
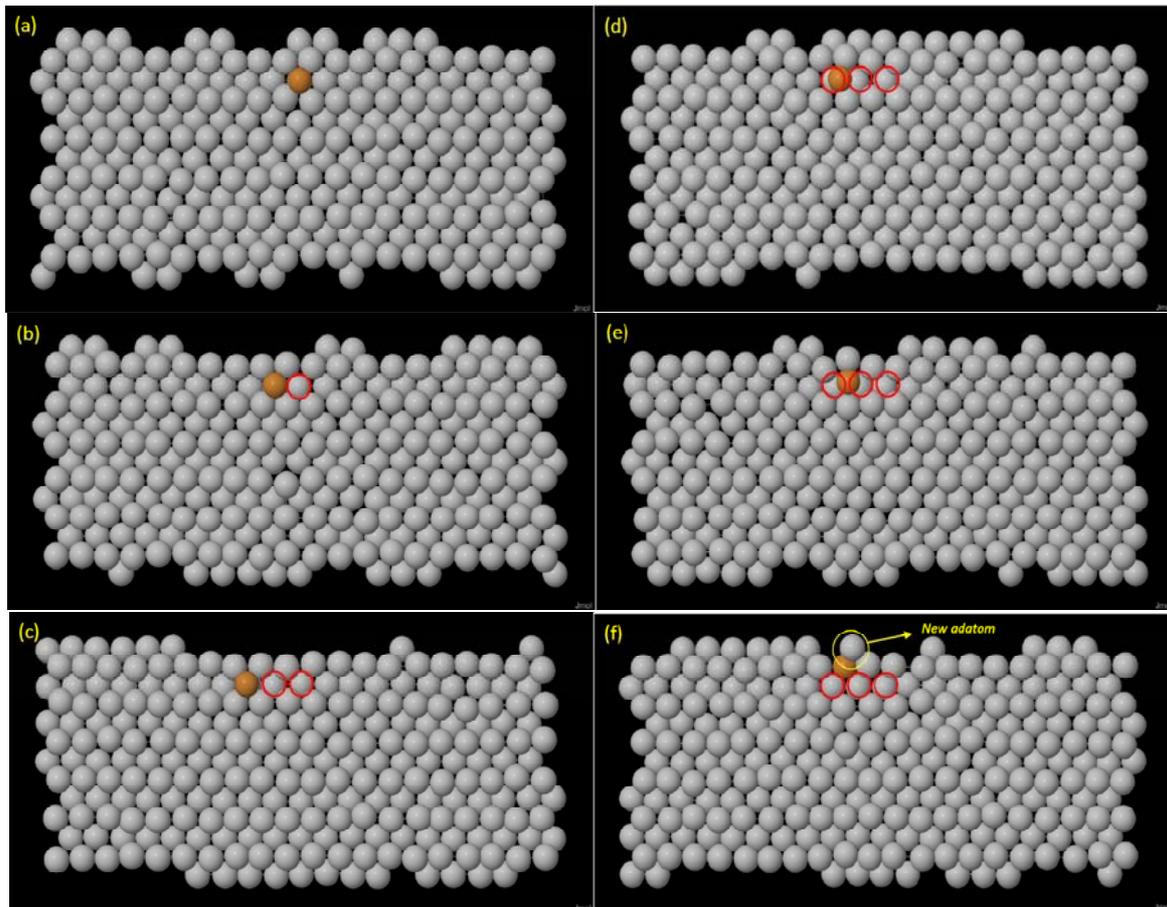

Fig. 1. the coexistence of jump process and exchange mechanism at 325 K. Figures a, b and c present the Cu adatom diffusion making simple jump, the red circles show the initial position occupied by the adatom in channel. The exchange process is presented by figures d, e and f where we note the apparition of new adatom (silver adatom).

Three different steps of molecular dynamics simulations were made to simulate our system. First, the simulation of adatom diffusion was started from the unrelaxed position of atoms. Due to the interatomic interactions, the system is allowed to relax to the minimum energy configuration. After relaxation, the system must be equilibrated at desired temperature keeping constant the number of atoms, the volume and the temperature. Finally our main program was run.

The first step in studying of adatom diffusion is the determination of saddle point or the static energy barrier that the adatom must overcomes (Table I). The results obtained by RGL [38], EA (AFW) [54], EA (VC) [54], CEM and MD-MC/CEM [55], and EM [56] were considered as reference for in-Channel jump. In order to

check the reliability of our results we have calculated the static energy barrier for both systems Ag/Ag(110) and Cu/Cu(110), which we have compared them with those obtained from others methods (See Table I). In Ag/Ag(110), EAM is in good agreement with all the available data for in-channel jump. In Cu/Cu(110), CEM and EA (VC) calculations give a much lower and higher barrier, respectively. Whereas, EAM is in a good agreement with RGL, EA (AFW), EM and MD-MC/CEM data. The static energy found in our systems is 0.27eV determined by the drag method where the number of free degrees was decreased by fixing the relaxation following x-direction and we left the system free to relax on 3N-1 directions.

Our previous work concerned mainly the study of the diffusion of Ag-adatom on Cu(110) surface [58] . Even if the Ag adatom jump process occurs mainly by simple jumps, the long jumps were also found to represent 4.23-12% of the total jumps.

Table 2. Adatom self-diffusion on the (110) surface. Single jumps represent the majority of jumps, a few multiple jumps are observed. S_j is the number of simple jumps, L_j is the number of multiple jumps.

	Cu/Ag(110)							
T(K)	305	310	315	320	325	350	375	400
S.T(ns)	30	30	30	30	30	30	30	30
S_j	68	80	95	76	88	50	122	107
L_j	0	1	1	1	2	0	0	0

The Ag adatom can reach the second, third, fourth and sometimes the fifth neighbour site in the same diffusion channel. This diversity of kind in jump process is due to the weakness of the in-channel diffusion barrier (Table 1).

The Ag adatom diffusion follows Arrhenius behaviour in a wide range of temperature (300 to 500K) without any anomalies such as in Cu/Cu(110) [38] (between low and high temperature). The activation energy and the prefectors of jump rate deduced from the Arrhenius plot are E_D=(0.216±0.001)eV and σ_0 =4.4ps^{-1} respectively. The value of dynamic energy E_D is close the static one (0.24eV). A remarkable analogy [38] is observed when comparing both diffusion of Ag and Cu on Cu (110), we found that they have the same static barrier energy (see Table 1), the same prefactor of rate jump (σ_0=4.4 for Ag/Cu(110) and σ_0=4ps^{-1} for Cu/Cu(110) at low temperature). In Cu/Ag(110), investigated herein this work, the higher diffusion barrier stops the diffusion of copper adatom and pushes it to lie in their initial position. For this reason, less activity was observed compared to Ag/Cu(110) system, especially at low temperature. The contribution of long jumps is still insignificant even at high temperature and presents less than 2.22% of total jumps. The same observation is noted in Ag/Ag(110) where the fraction of long jump never exceeds 3% [59]. Fig. 1 presents the coexistence of simple jump (figures a, b and c) and the exchange process (figures d, e and f) at 325 K. As can be seen from the figure, the Arrhenius behaviour is perfectly obtained between 305K and 325K with E_D=(0.27±0.01)eV and σ_0=6.6ps^{-1} (see Fig. 2). In this case the model of migration taking place by activated jumps is appropriate. However when the temperature exceeds 325K, the Arrhenius behavior is certainly no more valid because of the strong contribution of exchange process, this is clearly seen from Fig. 2. In recent work [29] the authors have observed the same behavior in Cu/Ag(100). At high temperature the exchange occurs after some iteration step (some hundreds of ps) stopping

the jump process of Cu adatom on the surface. In Ag (110) surface, the average amplitude of vibration perpendicular to the channel of top-layer atoms increase when the temperature increase [60], therefore, the adatom is pushed in the perpendicular direction making an exchange process.

Another alternative to check the Arrhenius law, we consider the diffusion coefficient expression obtained within the jump-theory (Eq.4). If the adatoms jump only between nearest neighbour sites and if we neglect entropy contribution, the prefactor of diffusion coefficient D_0 should be of magnitude of $\approx 10^{-3}$cm^2/s [61]. In Ag/Cu(110) the activation barrier is E_D=0.23eV which is equal to the static energy barrier and the prefactor of diffusion coefficient is D_0=6.68 10^{-3}cm^2/s noting that all points are joined by the same slight.
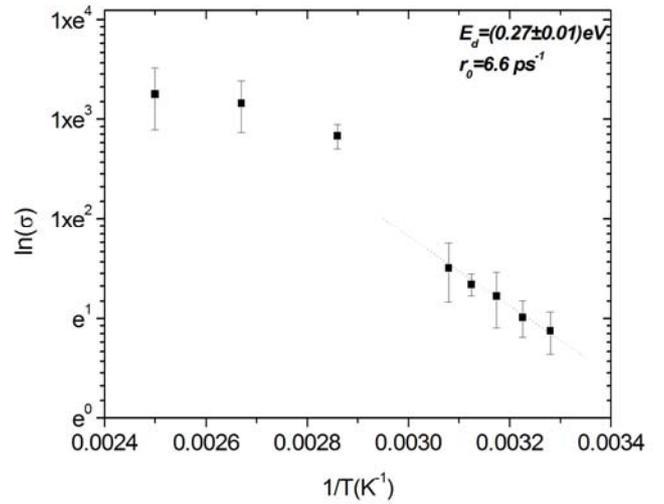

Fig. 2: Arrhenius plot of the in channel jump rate r_j

The dynamical barrier E_D=(0.29±0.01)eV calculated for Cu/Ag(110) from Fig. 3 is close to the value of static barrier mentioned before. The Arrhenius law is always satisfied at low temperature (less than 325K) with a diffusion coefficient prefactor D_0=6.68 10^{-3}cm^2/s. However when the temperature exceeds 325 K a significant deviations from the Arrhenius law occur. This anomaly proves that the diffusion becomes more complicated (correlation between processes), i.e the diffusion may become unactivated. To explain the difference between the adatom activity in Ag/Cu (110) [58] (where an important contribution of long jumps has been observed) and Cu/Ag(110), the dissipation parameter Δ on the easiest path (in-channel diffusion) was calculated. The one dimensional model of diffusion along the easiest was shown in a good agreement with the simulation [35] .The probability of long jumps depends on the energy dissipation parameter [62] where Δ is defined as follows:

$$\Delta = \frac{\eta}{k_B T} \int_0^a \sqrt{2m(U_s - U(x))}\, dx \qquad (6)$$

η presents the coupling friction between the adatoms and the substrate per unit mass and with δ-correlated noise [63] a is the long spacing along the direction path, U_s is the potential energy at the saddle point, and U(x) is the potential energy along the easiest path. If $k_B T \ll E_a$, where E_a is the activation energy or static energy barrier, then Δ can be given by:

$$\Delta \approx \frac{2\eta}{\pi k_B T} \sqrt{2mE_a} \qquad (7)$$

The friction can be related to autocorrelation function G(t) along the x direction by [64]

$$G(t) = \frac{1}{2} m \langle v_x(t) v_0(0) \rangle \qquad (8)$$

$$G(t) = A \exp(-\eta t/2) \cos(\omega t) \qquad (9)$$

with A=G(0)=k_BT/2. The velocity autocorrelation function G(t) at 400K versus time is represented in figure 4. The value of η was extracted by fitting the curves. For Ag/Cu (110), we find that $\eta \approx 2ps^{-1}$ and for Cu/Ag(110) $\eta \approx 11ps^{-1}$. Using Eq. (7), we can calculate the energy dissipation Δ for both systems and deduce that $\Delta_{Ag/Cu}/\Delta_{Cu/Ag} \approx 0.2$. The value of the ratio indicates that the dissipation of energy in Cu/Ag (110) is important than in Ag/Cu (110). We suggest that the few long jumps observed in Cu/Ag by comparison to Ag/Cu, can be explained physically by this effect of important dissipation energy in Cu/Ag.
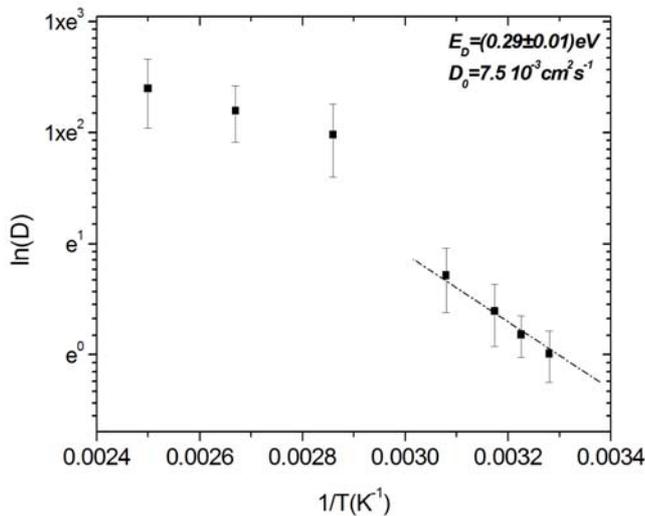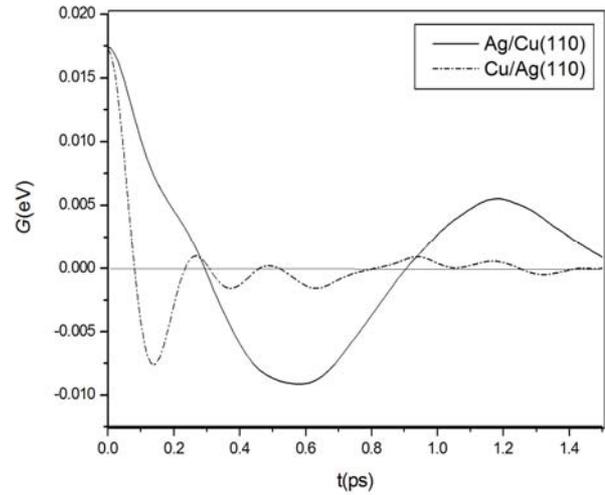

Fig. 4. The velocity autocorrelation function G(t) for the two systems. The dashed - dotted and solid lines correspond to Cu/Ag (110) and Ag/Cu (110), respectively.

3.2 Cross-channel diffusion

The diffusion of adatoms on metal surfaces may occur by different mechanisms; not only by simple or long jump, but also by exchanges process (see Figure 1 (d, e and f)). The presence of the exchange process has been shown Ag/Cu

Fig. 3. Arrhenius plot of the in channel coefficient diffusion D (10^{-7} cm^{2}s^{-1}). In Cu/Ag (110), some points come close to the straight (such at T=375 K).

Table 3. This table summarizes the static potential barrier

Exchange Process						
System	EA M	EA (AFW)	EA (VC)	RGL	EM	CEM, MD-MC/CEM
Ag/Ag	0.41	0.42(a)	0.31(a)	0.38(b)	0.56(b)	0.34,0.33(c)
Cu/Cu	0.29	0.30(a)	0.31(a)	0.29(b)	0.56(b), 0.26(e)	0.09,0.49(c)
Ag/Cu	0.32					
Cu/Ag	0.22					

(a)   From Liu et al. (Ref. [54])
(b)   From Montalenti and Ferrando (Ref. [38])
(c)   From Perkins and DePriste (Ref. [51])
(d)   From Slotz et al. (Ref. [56])
(e)   From Hansan et al. (Ref. [57])

(110) [58] and for different systems [30-33]. As bellow, the static barrier was calculated and compared to those existing in literature. All these values are summarized in Table 3.

Table 4: Adatom self-diffusion on the (110) surface. E_x is the number of exchange process. S.T : simulation Time (ns).

	Cu/Ag(110)				
T(K)	375	400	500	550	650
S.T(ns)	30	30	30	30	30
E_x	10	16	55	72	122

The drag method was used again to calculate the static barrier of exchange, but this time, by fixing the relaxation of the adatom in y-direction. From the energetic point of view, one may could predict that in channel diffusion would easy in Ag/Cu (E_{Jump} = 0.24eV (see Table I) and $E_{Exchange}$= 0.32eV (see Table III)) and the cross channel diffusion would be favorable in Cu/Ag (E_{Jump}= 0.27eV (see Table I) and $E_{Exchange}$= 0.22eV (see Table III)) but the coexistence of both process was obtained. As observed in Figures 2 and 3, the Arrhenius law is not respected when the temperature exceeds 325K, because of the occurrence of the exchange process which stops the adatom to make the in-channel diffusion. The statistical even of cross-channel diffusion at high temperatures (400 to 650 K) was summarized in table IV. The simulation time is extended to 30ns. Fig. 5 shows that the exchange process follows an Arrhenius law. This behavior was observed also in diffusion of copper adatom on Cu (110) [65]. By fitting the curve in Fig. 5, the dynamic barrier is found to be: E_{exch}=(0.21±0.01)eV which is close the static barrier and the prefactor $\sigma_0 \approx$ 2ps^{-1}.
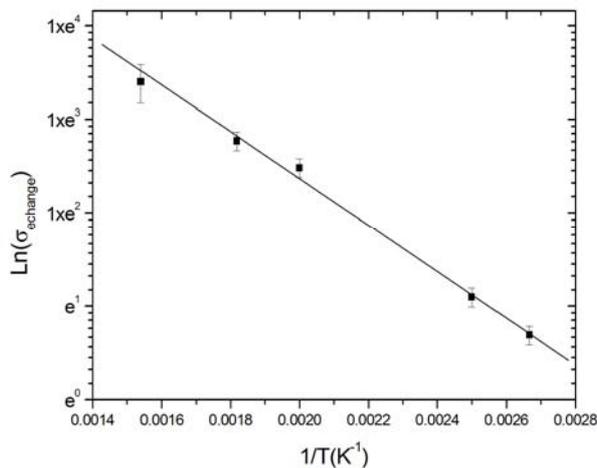

Fig. 5. In Cu/Ag and at high temperatures, the Arrhenius law of cross channel rate r_j is well satisfied (from 375K to 650K).

4. Conclusion

In this work we have studied the adatom diffusion using molecular dynamic simulation. The value of static barrier, calculated using EAM, is in a good agreement with the ones obtained by other method. The value of potential barrier calculated from the Arrhenius plot is close to the static energy barrier. In this study several phenomena have been observed and we note that the diffusion occurs in channel by jumps process (simple and double) and by exchange process. The Arrhenius law is perfectly satisfied at low temperature (less than 325K) for in-channel mobility and at high temperature (375 to 650K).The high energy dissipation of Cu adatom on Ag(110) surface, explains why we observe less number of long jumps than in Ag/Cu(110). Above 325K we cannot neglect an important phenomena such the exchange process which increases with temperature stopping the diffusion of Cu-adatom and lead to the deviation from the Arrhenius behavior as the result of a more complicated diffusion process.

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