



Effect of Substrate on Structural and Electronic Properties of Au-Pd, Au-Pt and Au-Ag Atomic Chains

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Authors' contributions

This work was carried out in collaboration between both authors. Author MRD designed the study, performed the Computation Work, Plotted the graphs and wrote the first draft of the manuscript. Author ACS managed the analyses of the study. Both authors read and approved the final manuscript.

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ABSTRACT

We report structure and electronic properties of Au-Pd, Au-Pt and Au-Ag bimetallic atomic chains absorbed on NiAl(110) and Cu(110) substrate. It is found that the presence of substrate significantly influences the electronic structure of the chains. Atoms of single chains of Au-Pd, Au-Pt and Au-Ag bind more strongly with Ni atoms of NiAl substrate, as compared with Cu atoms in Cu(110). The interaction between chain atoms is found stronger than the chain-substrate atoms, when chains are placed on Cu substrate, while it is other way round in case of chains on NiAl substrate. Effect of change in positions of atoms in bimetallic chains in presence of substrate is studied by placing double chains of Au-Pd, Au-Pt and Au-Ag on Cu (110) substrate in three different configurations. It is found that Au-Pd and Au-Pt bimetallic chains stabilize in double zigzag topology, when placed on Cu (110) substrate. While Au-Ag chains exhibit ladder topology on Cu(110) substrate. Ferromagnetism that is observed in ground state of free standing chains of Au-Pd and Au-Pt is not found when chains are absorbed on NiAl(110) and Cu(110) substrate. It is likely that the interaction between chain and substrate atoms results to zero magnetic moment.

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1. INTRODUCTION

One of the major goals of development of nanomaterials has been the understanding of how the system properties change on changing the structure of a material at atomic scale. Having known the interplay between structural, electronic, transport, and mechanical properties of atomic scale systems such as atomic chains, clusters, and nanowires makes it possible to manipulate different properties to design desired atomic scale devices [1-5]. As compared to bulk, atomic wires and clusters exhibit distinct reactivity, unveiling suitable chemical properties for catalysis applications [6,7]. Development of atomic wire systems is a step forward towards the ultimate miniaturization of electronic devices.

Two main experimental approaches have been implemented successfully to manufacture 1D structures. Formation of suspended metallic chains of heavy transition metals using mechanically controllable break junction experiments is one of the approaches [8-10]. Other approach is the manipulation of atoms on the substrate with the help of scanning tunneling microscope that make one to several atoms thick nanowires on the substrate [11-26]. Pioneering work by Nilius et al. [13] on Au and Au-Pd chains formed on NiAl(110) substrate has been followed by a series of theoretical studies to get insight into interplay between structure and electronic properties.[14-24] A complete series of reports by Miguel A have presented detailed study of bond formation and charge transfer mechanism for monomers and atomic chains of late transition elements [21-24]. The most recent report along these lines sheds light into change in structural and electronic properties, on alloying these atomic chains by single atom impurity of various elements [24]. It has been reported that in case of atomic chain made on a substrate, magnetism of chain is highly influenced due to the weak chain-surface hybridization [25-26]. For example, Heinze et al. displayed that free standing ferromagnetic Cr and Mn chains undergo the transition ferromagnetic to antiferromagnetic coupling when they are supported on Pd (110), Ag(110), and NiAl(110) surfaces [25].

Despite a huge number of studies on 1D atomic chains, two important aspects of atomic chains, which are least explored, are; (a) how presence of the substrates affect the structural, electronic and magnetic properties of bimetallic chains, and

(b) does alloying of a chain modifies the interactions between chain and substrate atoms. In our earlier studies, we investigated electronic, structural and magnetic properties of free standing bimetallic atomic chains of Au-Pd, Au-Pt and Au-Ag, using DFT based computations [27,28]. It was found that free standing atomic chains of Au-Pd and Au-Pt are magnetic and the magnetic moment depends on number and arrangement of Pd and Pt atoms in the chains. It has also been seen that the most stable free standing chain structures have zigzag geometry and exhibit metallic properties.

How the presence of substrate surface influences the electronic, structural and magnetic properties of chain motivated us to take up study of Au-Pd, Au-Pt and Au-Ag atomic chains deposited on NiAl and Cu surfaces.

NiAl(110) and Cu(110) surface are most widely and extensively studied for absorption of heavy 4d and 5d element.[13-26,29-32] However, there have not been many studies that illustrate how magnetic, electronic and transport properties of bimetallic chains change when chains on a substrate, as compared to free standing chains, are considered. In other words, to what extent electronic, magnetic and transport properties of a bimetallic atomic chain are modified due to the interactions between atoms of chain and substrate? Study of effects of the substrate on two different substrate which are most commonly used for fabrication of one dimensional structure is helpful in tailoring desired electronic, magnetic and transport properties.

In this paper, we report structural, electronic and magnetic properties of Au-Pd, Au-Pt and Au-Ag atomic chains formed on NiAl(110) and Cu(110) substrates. We compare our computed binding energy of chains on two substrate and find that total binding energy of all the three chains is higher for the case of NiAl(110) substrate, as compared to that for Cu(110) substrate. However, interaction of chain atoms with the substrate atoms is found higher for the case of chains formed on Cu (110) substrate. The computed projected density of states (DOS) shows strong interactions of d-orbital of Pd and Pt atoms of Au-Pd and Au-Pt chains with the d-orbital of Ni atoms of NiAl(110) substrate. While, Au atomic orbitals found to show almost no interaction with the Ni atoms. On the other hand Cu atomic orbitals, which are spread over wider

energy range, shows good orbital overlap with Au, Pd, Pt and Ag atoms. On comparing computed results on electronic and magnetic properties of chain-substrate systems with that of free standing chains, we find that the magnetic moment of Au-Pd and Au-Pt chains on NiAl(110) and Cu(110) substrate vanishes due to interaction of d-orbitals of Ni and Cu atoms with that of chain atoms. The paper is divided into four sections: Details of computation are reported in section-2. Our computed results are discussed in section-3, while conclusions are presented in section-4.

2. COMPUTATIONAL DETAILS

We performed our computations with the use of VASP code [33,34] that employs density functional theory (DFT), with projector-augmented wave (PAW) potential. [35] The exchange–correlation interaction between electrons are included through the spin-polarized generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) functional. [36] The valence electrons are described by a plane wave basis set using a kinetic energy cut-off of 450 eV. The Brillion zone for NiAl(110) and Cu(110) was sampled using a $6 \times 16 \times 1$ and $7 \times 16 \times 1$ k-points mesh, respectively, generated by the Monk horst–Pack

scheme [37] with 0.1 eV smearing width in Methfessel-Paxton method. Chosen K-points sampling and kinetic energy cut off provide convergence of 1 meV. Three-dimensional super cell having chain along z-axis and a large vacuum of 20 Å along x-and y-directions to separate the chain from periodic images and interaction has been chosen for performing computations. NiAl(110) substrate was modeled using four layers of (4×2) super cell. Cu(110) substrate was modeled using seven layers of (5×2) super cell.

Bimetallic chains of Au-Pd, Au-Pt and Au-Ag are modeled having alternating arrangement of Au and Pd(Pt, Ag) atoms. Chain atoms are placed on NiAl(110) and Cu(110) substrate along [001] direction on Ni and Cu bridge sites, respectively. On copper substrate in addition to chains having alternating arrangement of Au-Pd(Pt or Ag), two parallel chains structures of three possible arrangements are placed on Cu bridge site as shown in Fig. 1. To obtain relaxed geometry, first two layers of both the substrates of NiAl(110) and Cu(110) and atoms of chain were allowed to change position in Conjugate Gradient minimization scheme. Each chain/substrate system has been fully relaxed until the Hellmann-Feynman forces converged to a value less than 0.01 eV/Å per atom.

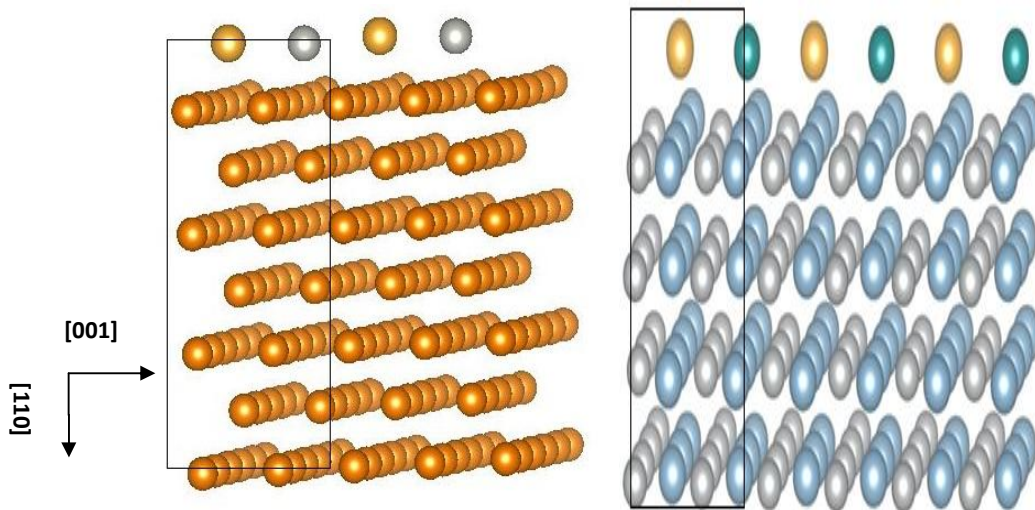


Fig. 1. Au-Pd, Au-Pt and Au-Ag chains over Cu (110) substrate (left side figure) and NiAl(110) substrate (right side figure). The copper atoms are represented by reddish yellow spheres. Al atoms are shown by light blue spheres while light grey spheres display Ni atoms in NiAl substrate. The chains atoms are shown by blue (Pd (Pt, Ag)) and yellow (Au) spheres, respectively, when are placed chain on substrates. The rectangle is the supercell used for the calculation

3. RESULTS AND DISCUSSION

As compared to free standing bimetallic chains, substrate-chain (bimetallic) system is expected to have increased metal-metal interactions. In order to study the effect of increased metal-metal interactions on the structural, electronic and magnetic properties of chains on a substrate, we modeled two parallel chains of each of Au-Pd, Au-Pt and Au-Ag on the substrates of NiAl(110 and Cu(110). When two parallel chains are placed on the most stable Ni-bridge sites of NiAl(110) substrate, the distance between the two chains is found larger to observe any notable interaction between the chains. In view of this, we have modeled a two chain system placed on Cu(110) substrate only. We further found that there can be three possible configurations for arranging two bimetallic chains on Copper substrate. These are displayed in the right panel of Fig. 2 and are termed as A, B and C types.

3.1 Structure and Stability

3.1.1 Single chains on NiAl(110) and Cu(110) substrate

To study how presence of substrate influences the structural properties of bimetallic chains, we compare our computed structure parameters of chains made on NiAl(110) and Cu(110) substrates with those of free standing atomic chains. It has been affirmed from several past studies that in case of NiAl(110) surface, Ni

bridge site is energetically more favourable as compared to Al bridge site [21-24], and [001] is favoured direction for growth of a chain [21-24]. Ni bridge sites on NiAl(110) surface provides a spacing of 2.89 Å along [001] direction for chain formation, which nearly matches with the nearest neighbour distance in bulk structures of Au, Ag, Pd and Pt. The nearest neighbour distances in bulk structures of Au, Ag, Pd and Pt bulk structure are; 2.88 Å, 2.89 Å, 2.75 Å and 2.77 Å, respectively. Like NiAl(110) substrate, the [001] is the most favoured direction of growth Cu(110) too [29,30,32]. The available spacing for placing the chain atoms along [001] direction is 2.54 Å in case of Cu(110) substrate, which is not very different from interatomic distance for free standing linear chains of Au-Pd (2.50 Å), Au-Pt (2.51 Å) and Au-Ag (2.62 Å).[38].

We find that the Pristine chains of Au, Ag, Pd and Pt make linear structure over the substrate. However alloyed chains of Au-Pd, Au-Pt and Au-Ag do not exhibit linear structure when placed on NiAl(110) and Cu(110) substrate. The alloy chains make a zigzag structure that slight deviates from linearity. The deviation is denoted by the angle ϕ for NiAl substrate and θ for Copper substrate, which are reported in Table 1. The deviation from linearity can be attributed to the difference in atomic radii of alloy atoms, Au, Pd, Pt and Ag. Because of this difference in atomic radii, each of these atoms in alloy sits at different heights on the Ni or Cu troughs, which results into zigzag geometry of bimetallic chains.

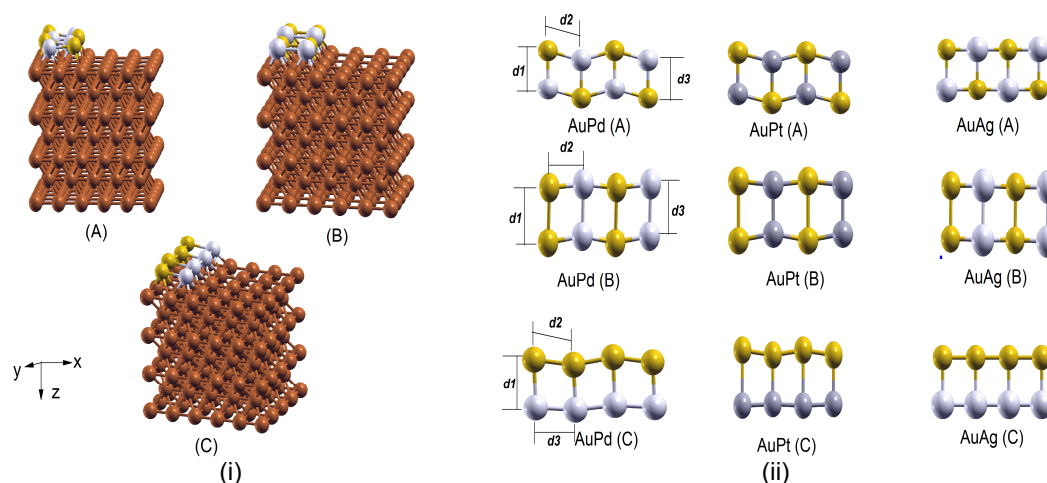


Fig. 2. (i) Three different configurations, termed as A, B & C, of Bimetallic chains placed on Cu(110) substrate. Relaxations of chain and substrate system yields three different possible configurations termed as A, B & C (ii) Enlarged forms of chains without substrate are shown. Grey atoms represent Pd(Pt, Ag), while Au atoms are shown by yellow spheres

Table 1. Our computed inter atomic distances (d), bond angle (ϕ, θ), for the single chain placed on NiAl(110) and Cu(110) substrate respectively are reported here. Magnetic moment of free standing chain (μ) is also listed in the table

	dAl-Au (Å)	dNi-Au (Å)	dCu-Au (Å)	dAl-Pd(Pt, Ag) (Å)	ddNi-Pd(Pt, Ag) (Å)	dCu-Pd(Pt, Ag) (Å)	ϕ	θ	μ (μ B/atom)
AuPd	2.76	2.58	2.65	2.65	2.55	2.57	178°	174°	0.42
AuPt	2.80	2.59	2.68	2.58	2.54	2.53	173°	170°	0.62
AuAg	2.79	2.57	2.65	2.92	2.62	2.72	174°	175°	-

Table 2. Computed values of E_{C-S} and E_{C-C} for single chains on NiAl(110) and Cu(110) substrates shown Fig. 1

	E_B (eV/atom)	E_{C-S} (eV/atom)	E_{C-C} (eV/atom)
NiAl + AuPd	-3.55	-2.39	-1.17
NiAl + AuPt	-4.38	-2.88	-1.50
NiAl + AuAg	-2.88	-1.53	-1.35
Cu + AuPd	-3.43	-1.96	-1.47
Cu + AuPt	-3.86	-2.33	-1.53
Cu + AuAg	-2.79	-1.32	-1.47

The interatomic distance between chain atoms and substrate atoms along with interaction energy and PDOS give an idea about nature of bonding and comparative strength of the bonding. A stronger bond has shorter interatomic distance, higher binding energy and better orbital overlap.

Observing interatomic distance of chain atoms and substrate atoms from Table 1 it can be said that AuPt chains bonds most strongly with the substrate compared to AuPd and AuAg chains.

Stability of a structure is described in terms of Binding energy (E_B) and interaction energy of the structure. The E_B can be expressed as sum of two contributions coming from chain-substrate E_{C-S} , and chain-chain, E_{C-C} interactions. Thus ; $E_B = E_{C-S} + E_{C-C}$, where

$$E_{C-S} = \frac{E_{tot} - E_{surf} - E_{adats}}{N_{at}} \quad (1)$$

$$E_{C-C} = \frac{E_{adats} - N_{at} \times E_{adats}}{N_{at}} \quad (2)$$

Our computed values of E_{C-S} and E_{C-C} for various chain configurations use of Eqns.(1) and (2) are reported in Table 2, which is given below :

As is seen from Table 3, the chain-substrate interaction energy (E_{C-S}) shows higher magnitude when NiAl(110) substrate is taken in place of Cu(110) substrate. The bond formation of Au-Pd, Au-Pt and Au-Ag atoms in the chains is stronger

with Ni atoms of NiAl(110) substrate, as compared to that with Cu atoms in Cu(110) substrate. Further, among the three bimetallic chains, Au-Pt chain exhibit highest magnitude of binding energy, followed by Au-Pd and Au-Ag chains in both the cases of substrates. We find this consistent with the past calculations on single atom chains of Pt, Au, Pd and Ag made on NiAl(110) and Cu(110) substrates [23]. It has been found that the tendency of chain formation is highest for Pt followed by Au, Pd and Ag atoms. It is to be noted from Table 3 that except Au-Ag chains on Cu(110) substrate, all other bimetallic single chains on a substrate show smaller magnitude of E_{C-C} than that of E_{C-S} , suggesting a stronger interaction between atoms of chain and substrate, rather than interaction between the atoms of a chain. Another important observation that can be made from Table 2 is that bimetallic chains bind more strongly with NiAl(110) substrate than that with Cu(110) substrate.

3.1.2 Double zigzag chains on Cu(110) substrate

We also studied the change in structure and energetics for a system of two parallel chains of Au-Pd, Au-Pt and Au-Ag placed over copper substrate. As is shown in Fig. 2, two single chains can be placed on copper substrate in three different manners. After relaxation of chain-substrate system, we found that double zigzag structures or ladder structure geometries

emerge, depending on the configuration of atoms, which are depicted in the figure.

The interatomic distances d_1, d_2 and d_3 , and the bond angle θ , which characterize the equilibrium geometries shown in Fig. 2, are reported in Table 2. The d_1 and d_3 denotes the distance between atoms of two different chains, while d_2 represents the distance between atoms of the same chain. Since the atoms of the same chain occupies equivalent Cu bridge sites, is found almost same for all structures and it is of the order of supercell parameter 2.54 Å for most of the structures. However, d_2 values are larger than 2.54 Å (<2.64 Å) for A-type structures of AuPd (2.64 Å) and AuPt-A (2.63 Å). This increased value of d_2 is responsible for the double zigzag geometry of the A-types of AuPd and AuPt chains over Cu(110) substrate as can be seen from Fig. 2.

Our computed values of E_B , E_{C-C} and E_{C-S} for double zigzag structure chains over Cu(110) substrate are given in Table 4. As is seen from the table, binding of chain atoms with substrate is strongest in case of Au-Pt and weakest for Au-

Ag. Also, chain-chain atoms bind more strongly than chain-substrate atoms. We also notice from table that for all three cases of Au-Pt, Au-Pd and Au-Ag, binding energies show the trend; type-A>type-B>type-C suggesting that the type-A structure are most stable.

3.2 Electronic and Magnetic Properties

Strength of a bond can be deduced from the projected density of states (PDOS) plots. Major overlap of orbitals indicates a stronger covalent character of the bond. Our computed PDOS of bimetallic chains on NiAl and Cu substrates are plotted in Figs. 3 to 6. These figures also exhibit the PDOS for free standing chains of Au-Pt, Au-Pd and Au-Ag. On comparing PDOS of chain over substrate with those of free standing chains, we find that the PDOS, which are confined to narrow energy range with higher peak values in case of free standing chain, are transformed to those that have enlarged energy range and smaller peak heights when chains are formed on the substrates. It suggest suggests that the one dimensional character that is observed electronic properties of free standing atomic chains tends to quasi-one dimensional when chains are placed over the substrate.

Table 3. Inter atomic distances (d_1, d_2 & d_3), and bond angle (θ), for double zigzag chains on Cu(110) substrate , which is exhibited in Fig. 2

	$d_1(\text{Å})$	$d_2(\text{Å})$	$d_3(\text{Å})$	θ	μ ($\mu\text{B}/\text{atom}$)
AuPd (A)	2.78	2.64	2.78	148°	0.23
AuPd (B)	2.90	2.55	2.71	170°	0.05
AuPd (C)	2.74	2.56	2.55	163°	0.23
AuPt (A)	2.81	2.63	2.81	150°	0.41
AuPt (B)	3.17	2.56	2.61	166°	0.08
AuPt (C)	2.77	2.56	2.54	167°	0.09
AuAg (A)	2.84	2.54	2.84	178°	-
AuAg (B)	2.84	2.55	2.91	170°	-
AuAg (C)	2.90	2.54	2.54	179°	-

Table 4. Computed values of E_{C-S} and E_{C-C} for double zigzag chains/Cu(110) system as exhibited in Fig. 2

	$E_B(\text{eV}/\text{atom})$	$E_{C-S}(\text{eV}/\text{atom})$	$E_{C-C}(\text{eV}/\text{atom})$
Cu + AuPd (A)	-3.49	-1.51	-1.98
Cu + AuPd (B)	-3.45	-1.55	-1.89
Cu + AuPd (C)	-3.41	-1.43	-1.98
Cu + AuPt (A)	-4.25	-1.73	-2.52
Cu + AuPt (B)	-4.23	-1.63	-2.60
Cu + AuPt (C)	-4.19	-1.68	-2.51
Cu + AuAg (A)	-2.81	-1.06	-1.75
Cu + AuAg (B)	-2.81	-1.13	-1.68
Cu + AuAg (C)	-2.78	-1.12	-1.66

From the plots of PDOS, we also observe a significant reduction in orbital overlap in atoms of chain, when chains are formed on substrate, rather than taking these as free standing chains. The reduction in overlap of atomic orbitals, for chains on substrates, is an indication of the weakening of bond strength between chain atoms. In case of chain on substrate, interaction of chain atoms with substrate atoms are found stronger, as compared to that between atoms of chain. We further find that the magnetic moment observed in free standing chains of Au-Pt and Au-Pd is not seen when these bimetallic chains are formed on NiAl(110) and Cu(110) substrates. The important transition from magnetic state to non-magnetic state can be understood from two changes that are observed in DOS plot: (i) Shifting of d-band edge away from Fermi level, and ii) stronger interaction of Pd/ Pt atoms in chain with the Ni/Cu atoms of the substrate, as compared to interaction between Au and Pd or Au and Pt atoms. Shifting of d-orbital away from

Fermi energy in chain-NiAl system lowers the total density of states at Fermi level, and neutralize spin polarization originated from reduced dimension of Pd and Pt d-orbital.

3.2.1 Single chains on NiAl(110) and Cu(110) substrate

Fig. 3 compares PDOS of single chains of Au-Pd, Au-Pt and Au-Ag on NiAl(110) and Cu(110) substrates with that of free standing chains. On comparing PDOS of Au, Pd, Pt & Ag atoms with those of Ni, Al and Cu in substrates, we find that there is minimal overlap between Au atoms and substrate atoms. On the other hand, Pd and Pt atoms show larger overlap of orbitals with the substrate atoms. For example, in case of Au-Pd chains placed on NiAl(110) substrate, Pd atoms show highest overlap with Ni atoms, while Au atoms show negligible overlap with Ni and Al atoms. While, Au and Pd atoms shows good overlap with Copper atoms of Cu(110) substrate.

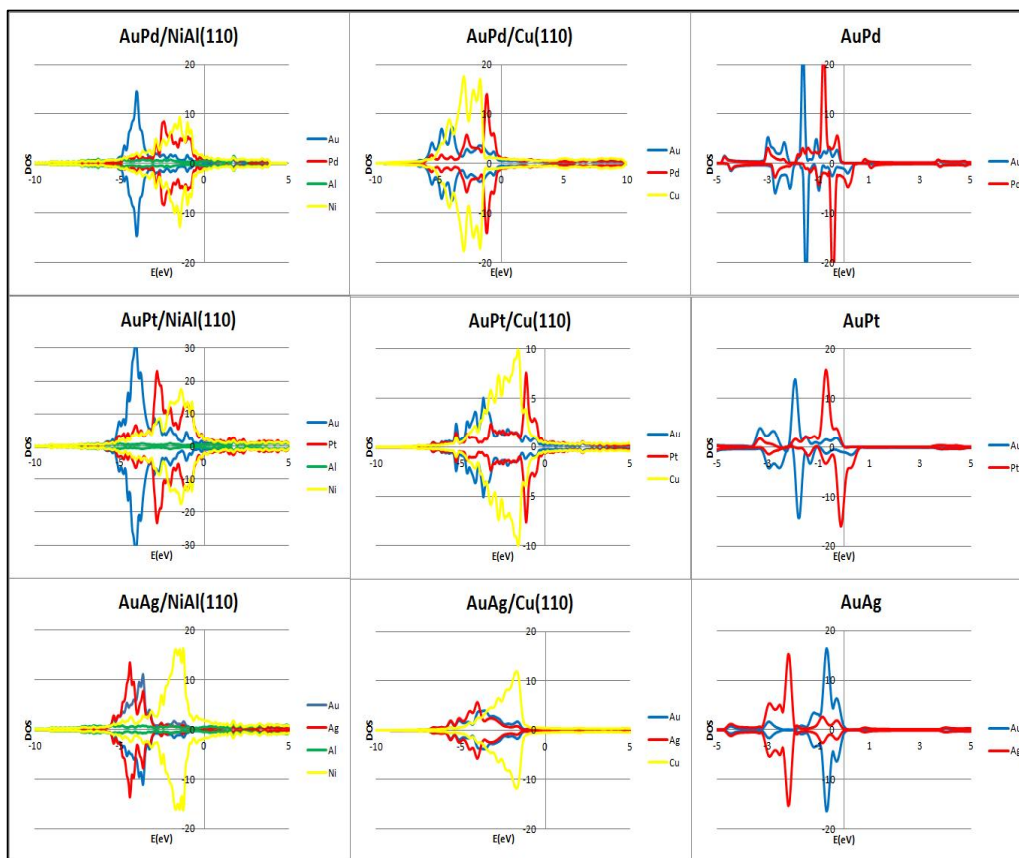


Fig. 3. Projected density of states (PDOS) are plotted as function of energy for chain-NiAl(110), chain-Cu(110) systems. The PDOS for free standing chains of Au-Pd, Au-Pt and Au-Ag are also displayed in the figure

On comparing PDOS of Au-Ag chains in presence and absence of the NiAl(110) and Cu(110) substrate, it is clearly seen that Au and Ag atoms of the Au-Ag chains have good orbital overlap in presence of NiAl(110) and Cu(110), while free standing Au-Ag chains exhibit small orbital interaction. We can thus infer that presence of substrate enhances Au-Ag chain formation possibility.

In our earlier work on free standing bimetallic chains [28] we found that free standing chains of Au-Pd and Au-Pt are magnetic and the magnetic moment depends on the interatomic distance. In this paper, to find the effect of substrate on the magnetism of a chain, we performed spin polarized calculations in presence and absence of NiAl(110), and Cu(110) substrates for the cases of Au-Pd and Au-Pt chains. It is observed that in presence of the substrate the chains lose its magnetism. The magnetic moment per atom of free standing single chains of Au-Pd and Au-Pt

are reported in Table 1. Here, we would like to notify that the magnetic moments of the chains, in absence of the substrate, is not computed for the ground state of the freestanding chains but it is computed with the same interatomic distance, as is in the chains on the substrate, which is larger than the ground state interatomic distances.

3.2.2 Double zigzag chain on Cu(110)

Figs. 4 to 6 display PDOS of Au-Pd, Au-Pt and Au-Ag chains, respectively, on Cu(110) substrate for three different configurations (A,B &C) that are shown in Fig.1. Like the case of single chains, a refitting of PDOS from Fermi energy is observed when double zigzag chain structures are placed on copper substrate. This refitting of PDOS results into lesser number of states near the Fermi energy for the chain substrate system, as compared to free standing chains.

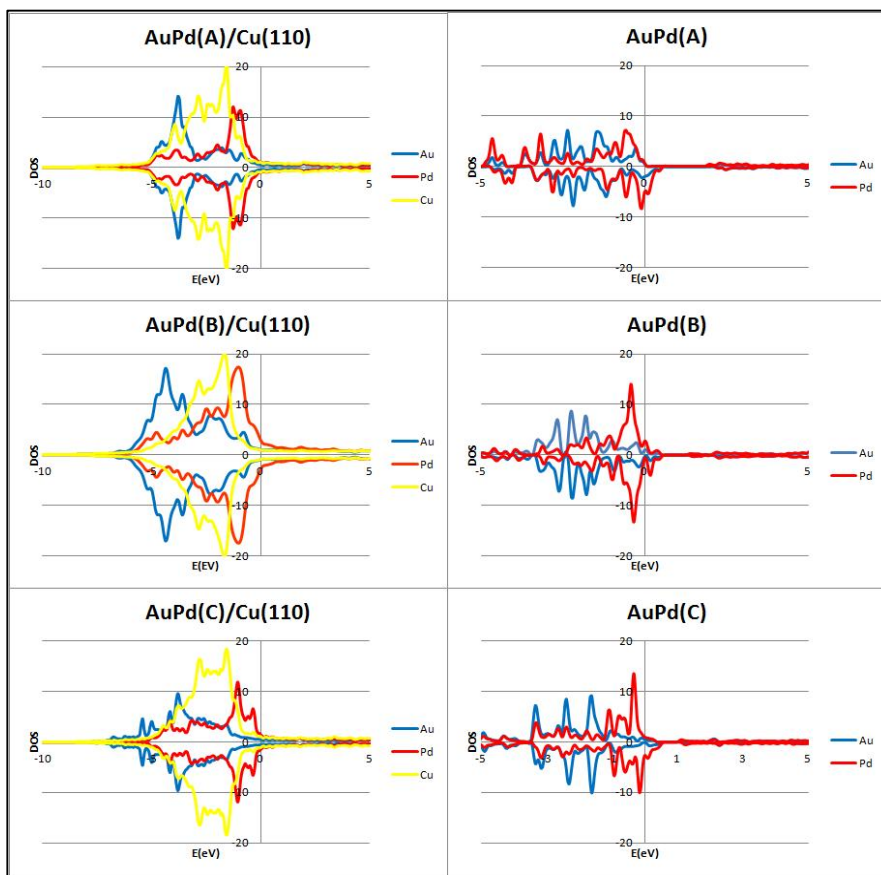


Fig. 4. PDOS for different configuration of Au-Pd double zigzag chains on Cu(110) substrate (left panel) and corresponding free standing chains of Au-Pd(right panel). The structures are exhibited in Fig. 2

It is interesting to note that on comparing different properties of bimetallic chains; we find that the computed binding energies of the A, B and C configurations do not differ much from each other, while computed PDOS plots of one structure significantly differ from those of other structures. Fig. 4 shows PDOS of three types of Au-Pd chain configurations on Cu (110) substrate. As is noticed from the figure, overlap of orbitals is more in case of type-C structure as compared to types A and B configurations. This trend is very different from that observed in case of free standing chains, where orbital overlap of Au and Pd(Pt, Ag) atoms found larger in type-A; followed by type-B and type-C configurations. Considering alloying point of view, type-A shows highest degree of alloying, followed by type-B and type-C.

Similar trend is observed in case of Au-Pt chains on Cu(110) substrate, as is seen in Fig. 5. When chains are placed over Cu(110) substrate, Cu-atoms exhibit stronger bonding with the Pd and Pt atoms in the Au-Pd and Au-Pt chains, as compared to the bonding between different

atoms in double zigzag chains of Au-Pd and Au-Pt. On comparing interaction among various atoms of bimetallic chains on Cu(110) substrate, we find that Au-Ag chains shows stronger tendency of alloying in presence of the substrate. As is seen from Fig. 6, there is very good orbital overlap of Au and Ag atoms for all the three types in case of Au-Ag double chains placed on Cu(110) substrate. It can therefore be inferred that different types of atoms in chains exhibit weaker bonding among themselves, as compared to their bonding with substrate atoms in case of double zigzag structures over the substrate.

Our computed PDOS for types A, B and C of double zigzag chains of Au-Ag on Cu (110) substrate are plotted in Fig. 6. On comparing Figs. 4 to 6, we find that the most stable alloyed double zigzag chain structure on Cu (110) substrate appears for the case of Au-Ag. Also, the comparison between double zigzag and single chains formed from Au-Ag atoms over Cu (110) substrate, it is found that double zigzag structures are fairly stable.

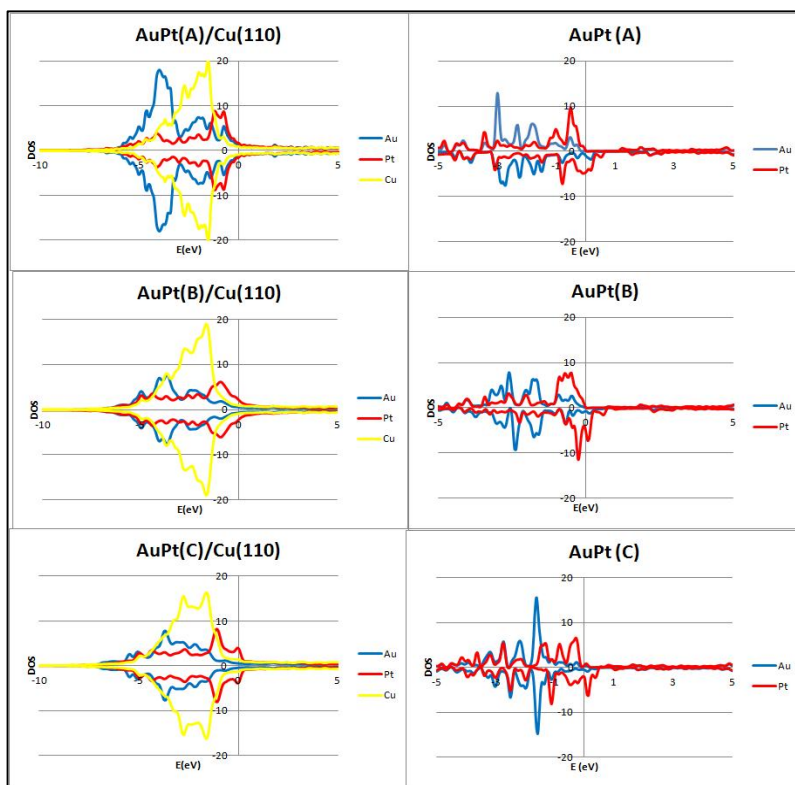


Fig. 5. PDOS for different configurations of Au-Pt chains on Cu(110) substrate (left panel) and for corresponding free standing chains of Au-Pt(right panel), whose geometries are as shown in Fig. 2

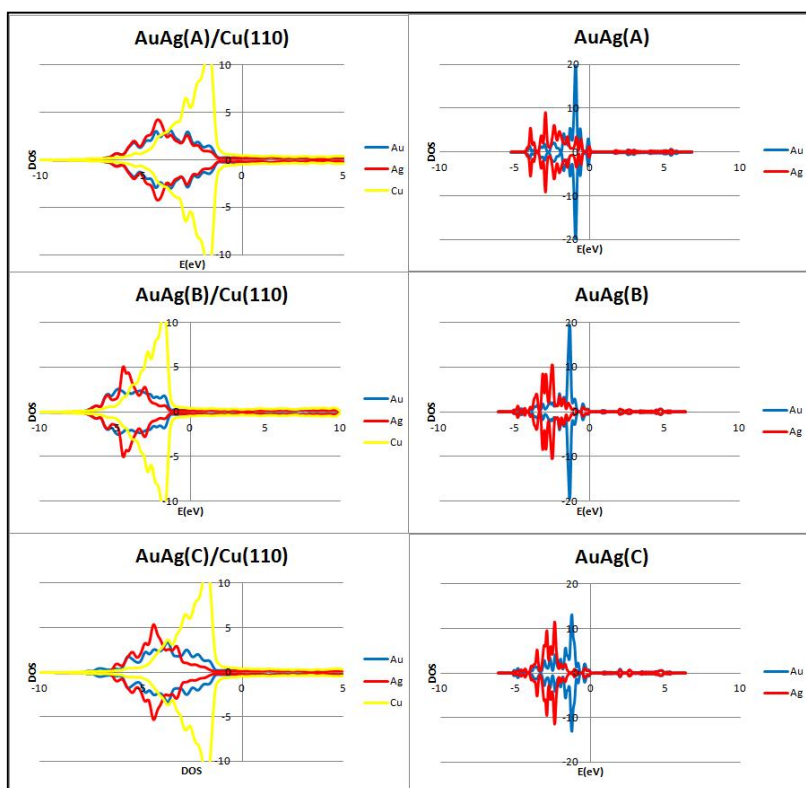


Fig. 6. PDOS for different configuration of Au-Ag chains on Cu (110) substrate (left panel) and for corresponding free standing chains of Au-Ag (right panel). The geometries of structures are shown in Fig. 2

It is found that the magnetic moment for both single chain and double chains on the substrate are zero. Unlike the case of single chains on the substrate, where E_{C-C} is lower than E_{C-S} , one can expect a nonzero magnetic moment for double chain structure on substrate. Because, in the case of double chains on Cu(110) substrate, chain atom interaction energy, E_{C-C} is higher than Chain-Substrate interaction energy, E_{C-S} as seen from Table 4. Thinking that the cancellation of magnetic moment is resulted from higher chain-substrate interaction, we expected some magnetic moment for the cases of double chains on Cu (110) substrate. However, we do not observe any magnetic moment for all the three configurations of types A,B and C of the double chains of Au-Pd and Au-Pt.

4. CONCLUSION

To summarize, we studied structure and electronic properties of bimetallic chains of Au-Pd, Au-Pt and Au-Ag on two different substrates of NiAl(110) and Cu(110). It is found that the presence of NiAl and Cu substrates significantly

influences the electronic structure of the chains. Atoms of single chains of Au-Pd, Au-Pt and Au-Ag bind more strongly with Ni atoms of NiAl substrate, as compared with Cu atoms in Cu (110). The interaction between chain atoms is stronger than the chain-substrate atoms, when chains are placed on Cu substrate, while it is other way round in case of chains on NiAl substrate. On comparing PDOS and interaction energy of free standing chains of Au-Ag with that of chains placed on the substrate, we find that presence of substrate induces bond formation between Au and Ag atoms which are otherwise not possible in free standing situation.

Another significant change in the presence of the substrate is shifting of d band away from Fermi energy. To study further the effect of increased chain atom interaction, we placed two chains on Cu (110) substrate in three different combinations, termed as A, B and C. It is found that, Au-Pd and Au-Pt bimetallic chains are stabilize in double zigzag topology, when placed on Cu (110) substrate. While Au-Ag chains exhibit ladder topology on Cu (110) substrate.

The comparison of computed binding energy of three structures, we find that A- type atoms have higher binding energy, as compared to B and C types, when placed on the substrate. Our calculations also show that the magnetic moment of the chain atoms vanish in presence of the substrate. Our plots of interaction energy and PDOS suggest that the magnetic moment is cancelled out due to two reasons; (i) stronger interaction of Pd(Pt) atoms with that of the substrate, and (ii) shifting of orbital away from fermi energy

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COMPETING INTERESTS

Authors have declared that no competing interests exist.

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