



Unveiling processing-structure-property correlations in SiO₂-Cr-Au composite thin films from molecular dynamics simulations

Tejasva Vashistha^a, Kishalay Raj^a, Harshit Kumar Gupta^b, Raghavan Ranganathan^{a,*}

^a Department of Materials Engineering, Indian Institute of Technology Gandhinagar, 382055, India

^b Inertial Sensors Entity, ISRO Inertial Systems Unit, Trivandrum, Kerala, India

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ABSTRACT

Precisely-engineered thin films are essential for many technological applications such as coatings, sensors and semiconductor devices. Since the microstructure of thin films, and thereby, their functionality is shaped by the processing conditions, it is imperative to comprehend the relationship between processing, structure, and the resultant properties. Thin films of chromium and gold are employed in precision accelerometers in autonomous navigation and guidance of missiles and launch vehicles. Performance of these thin films is dependent on the stability of thin films deposited on the non-metallic, highly stable pendulous structure made of fused silica. The purpose of this work is to investigate the connection between thin film processing parameters, microstructural features, and the mechano-thermal properties of Cr-Au thin films deposited on fused silica using Molecular Dynamics (MD) simulations. Simulations mimic the sputtering phenomenon over a range of deposition energies, followed by annealing, to unravel the structural changes, defect features and ensuing properties such as Young's modulus, compressive strength, hardness and coefficient of thermal expansion. We show that moderate deposition energies and lower annealing temperatures are crucial for enhancement in modulus, strength and hardness, while lower deposition energies result in structures possessing larger toughness.

1. Introduction

Thin film growth on substrates has become an area of current interest in materials engineering. Thin films are materials ranging from a few nanometers to several micrometers in thickness, deposited on various surfaces to modify its properties [1]. Sputtering is a popular thin film deposition technique that involves removing atoms from a solid cathode by means of incoming ions striking it. The deposition rate and incident energy of the target material on the substrate can be regulated by changing the incident ion energy. Sputter damage is a phenomenon that can occur when the incident ion energy is too high [2,3]. This can result in issues with film quality such voids and vacancy creation, as well as possibly causing the deposition process to fail. Film quality is generally impacted by deposition rate as well [3–5]. Therefore, for better insight into the mechanisms of defect growth as well as for practical film quality control, it is crucial to understand the relationship between the morphologies of growing thin films and various sputtering process parameters.

Metal films find extensive use in power devices, semiconductors, micro-electro-mechanical systems, and sensors [6–9]. Films with

outstanding mechanical, electrical, and optical stability, as well as thermal and chemical stability, are needed for these technologies [10, 11]. Strong adherence to the substrate material, superior electrical conductivity, and consistent thickness are often traits of premium metal films. Thin films deposited on a pendulous non-metallic structure of precision accelerometers (see Fig. 1) is one such niche application finding wide application in field of autonomous Inertial Navigation Systems (INS). The stability of the pendulous structure, made of highly stable fused silica (SiO₂) on which the thin film is deposited, dictates the performance of accelerometers and thus, the INS. The purpose of the thin film deposition here is mainly to act as an electrode for the measurement of capacitance change resulting due to the movement of pendulum in response to the inertial acceleration experienced by the casing of the device. Here, thin film should not add any additional stiffness or variable forcing function on the structure like residual stress relaxation, thermal effects, creep phenomenon, etc. Hence, it is essential to characterize the ensuing thin films and understand the parameters affecting the stability and properties of the films.

It is also essential in some applications to guarantee the film's mechanical stability [12]. Noble metal films, which include gold, silver,

* Corresponding author.

E-mail address: rraghav@iitgn.ac.in (R. Ranganathan).

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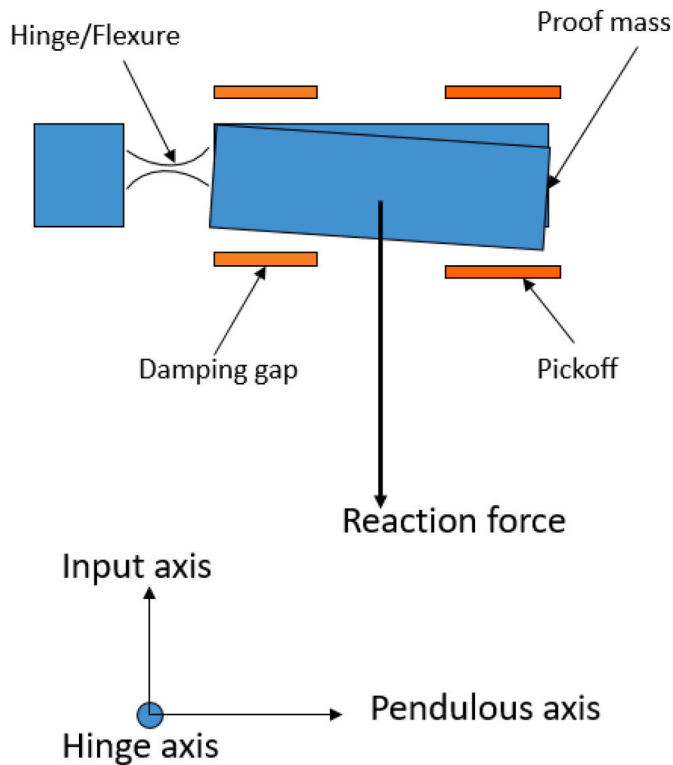


Fig. 1. Schematic of a precision accelerometer containing a thin film metallic coating on an Inertial Navigation System. Reaction force and the damping gap for the divide are indicated.

and platinum, have garnered significant interest because of their possible uses and minimal chemical reactivity. Because of its excellent chemical stability and electrical conductivity, gold (Au) is a highly valued film material in real-world applications [12,13]. But Au's low chemical reactivity prevents it from attaching well to oxide substrates like fused glass. One popular technique for improving the adherence of gold films to oxide substrates is the use of a metal adhesion layer. The most often employed substance for the adhesive layer is chromium (Cr), because to its higher chemical reactivity than noble metals [14]. Cr has the capacity to chemically attach to the substrate, enhancing the overlayer's adhesion and thermal stability. In semi-conductors, the chromium-gold (Cr/Au) bilayer is commonly used [15]. The thickness of chromium and gold for deployment in accelerometers is selected such that its impact on structural aspects of the parent structure does not get altered.

The substrate material is typically coated with metalized film layers using chemical or physical techniques. During deposition, the adhesion layer and the overlayer go through the processes of nucleation, grain development, and continuous film creation [11,16]. In addition, a multitude of crystal defects, including point defects and dislocations, may be present in the deposited layer because gaseous atoms lack the energy necessary for efficient diffusion into the substrate [17]. Increased internal stress caused by a higher fault density in the film could have a negative impact on the functionality of the device. In actuality, the annealing procedure is frequently employed to remove flaws from the film and enhance its characteristics.

SiO₂ is a versatile material known for its inert and stable nature, acting as an insulating layer with high thermal stability and transparency in the visible range, making it a popular substrate material due to its abundance and cost-effectiveness [18]. Vacuum evaporated SiO₂ thin films are crucial in optical device manufacturing, offering precise optical characterization through spectrophotometry and spectroscopic ellipsometry, revealing structural details and defect quantification [19].

Additionally, SiO₂ thin films prepared by dual ion-assisted deposition exhibit amorphous structures with varying properties based on deposition parameters, influencing refractive index, surface roughness, and microstructure density [20]. Chromium exhibits remarkable resistance to corrosion and oxidation, high hardness, and good adhesion properties [21]. It is also known for its moderate electrical conductivity, thermal stability, ease of deposition, and strong adhesion to substrates [22]. Gold (Au) is indeed highly resistant to corrosion and oxidation, malleable, ductile, and exhibits excellent electrical conductivity and stability [23, 24]. In the SiO₂/Cr/Au thin film composite structure, the adhesion, conductivity, and corrosion resistance of the Cr and Au layers are combined with the insulating, protecting, and optical qualities of SiO₂. This makes it an adaptable coating for a variety of uses, including microfabrication [18], optoelectronics [19], and packaging. Chu et al. [25] deposited a Cr-Au composite film on fused silica using electron beam evaporation and observed that the annealing temperature played a pivotal role in modulating the stresses, resistivity, mechanical properties and interdiffusion of Cr into the Au layer. In the work by Wang et al. [26], the shape and coverage of thin films produced by the sputtering technique were investigated using a three-dimensional molecular dynamics (MD) simulation. However, atomistic mechanisms responsible for the complex processing-structure-property relations remain elusive.

In this study, we employ molecular dynamics (MD) simulations to investigate the deposition behavior and study the thermo-mechanical properties of the SiO₂-Cr-Au composite structure. Our objective is to understand the structure and stresses developed during the thin film deposition on one hand and the properties (tensile and compressive behaviour, hardness and thermal expansion) on the other, and establish a correlation with the deposition parameters.

These films make it possible for devices used in seismic detection, automotive, aerospace, and structural monitoring to use capacitive sensing, electrode stability, and adhesion in environments possessing a wide range of temperatures (typically from -55°C to 125°C). State-of-the-art precision accelerometers are often subjected to a combination of extreme conditions such as vibrations from a few Hz to a few kHz 100 Hz and shocks that can reach 100g and beyond. A combination of high stiffness, large tensile strength and hardness and low thermal expansion are crucial for reliable functioning. The present work shows that under optimum processing conditions, one can achieve SiO₂-Cr-Au composite thin films possessing a combination of high stiffness, strength, compressive modulus, hardness and low thermal expansion, which is crucial for robust performance.

2. Computational procedure

This section describes the method for the generation of the amorphous substrate, the deposition process [27–29] and associated variables, the interatomic potentials used for describing all the interactions, and finally, the method for estimating thermophysical properties of the deposited thin films. All the simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) simulation package [30].

2.1. Interaction potentials

Table 1 provides details of the interatomic potentials employed to model both homonuclear and heteronuclear interactions within the system. These include *like* elemental interactions (e.g. Si-Si) and also cross interactions between atoms of the substrate and the deposited thin films. The parameters were chosen from prior works (see Table 1 for references) that have indicated a good reproduction of the respective material properties and interfacial behavior, critical to the fidelity of our simulations.

Table 1
Interatomic potentials for different atomic configurations.

Type of interaction	Interatomic Potential	Interaction Cutoff	References
Si-Si, O-O and Si-O	Tersoff	N/A	[31]
Au-Au	EAM	N/A	[32]
Cr-Cr	MEAM	N/A	[33]
Si-Cr	Morse	4.04	[34]
O-Cr	Morse	3.51	[35]
Cr-Au	Morse	2.74	[36]
O-Au	Lennard-Jones	4.29	[37,38]
Si-Au	Lennard-Jones	3.85	[37,38]

2.2. Amorphous silica substrate

To generate the amorphous silica substrate, a 7056-atom system of silica was chosen for melt-quench simulations. Initially, the β -cristobalite structure of crystalline silica was equilibrated at 300 K for 0.2 ns under fully periodic boundary conditions. The density was fixed at 2.17 g/cm^3 , corresponding to crystalline silicon dioxide (c-SiO₂). The Verlet algorithm was utilized to numerically integrate the equations of motion with a time step of $\Delta t = 1.0 \text{ fs}$. Interaction between silicon and oxygen was modelled using the Tersoff potential [39]. Initially, the crystalline SiO₂ sample was heated to $T = 5000 \text{ K}$, well beyond the experimental melting point of 1713°C [40] and was equilibrated at 5000 K for 2 ns using NVT ensemble.

Subsequently, the formation of an amorphous SiO₂ (a-SiO₂) structure was achieved by quenching the liquid to a final temperature of 300 K with a cooling rate of 11.75 K/ps (see Fig. 2). Finally, the structure was further equilibrated at 300 K for 0.2 ns .

2.3. Deposition of Cr and Au on silica

Before the deposition of the Cr and Au layers, the periodic silica box was first made non-periodic along the z-axis (by extension of the simulation cell length along z-axis) followed by a short relaxation of the structure to facilitate surface reconstruction [41]. The bottom ($0\text{--}8 \text{ \AA}$) along the z-axis of the silica substrate was held fixed, and the rest of the region ($8\text{--}30 \text{ \AA}$) was thermostatted [27–29,42] at 300 K . Subsequently, a moving deposition window of dimensions $48.5 \times 48.5 \times 20 \text{ \AA}^3$ was chosen in such a way that the height of this window always maintained at a constant distance from the growing instantaneous film surface. This was necessary to ensure that the velocity of all incoming atoms (which were integrated under NVE along with a Langevin thermostat) had a fixed average z-component towards the growing film (see Fig. 3). Initially, Cr, modelled using the EAM potential [43], was deposited on the silica

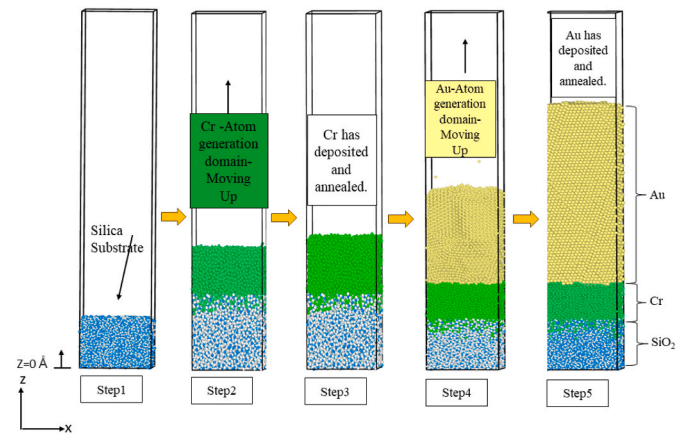


Fig. 3. Atomistic snapshots of the substrate and the deposition of Cr, followed by Au from a moving deposition domain. Color code: SiO₂ – blue and silver; Cr – green and Au – gold.

surface atom-by-atom from the moving window region. The starting position of the atoms was chosen using a random number. The components of velocity were chosen in such a manner that the z-component corresponded to a specified deposition energy ($20, 50$ or 100 eV), i.e., the z-component was a fixed negative value to make the atom deposit on the silica substrate, and the x and y components were allowed to range from a small negative to positive value, with a magnitude being a fraction of the z-component. This ensures growth of the thin film uniformly along the later axes, layer-by-layer. This was followed by the deposition of Au on the Cr surface using a similar protocol as above, and as shown in Fig. 3. The interatomic interaction between SiO₂ and Cr was modelled using the MEAM potential [44]. The thickness ratio of SiO₂ to Cr to Au was maintained as $1:1.33:4$, to mimic realistic experimental thickness ratios. The Si-Cr [34] and O-Cr [45] interactions were modelled using the Morse potential. Following deposition, the system was annealed at either 700 K or 1000 K to relieve stresses and to check the effect of annealing on thin film properties. It is to be noted that the deposition energy for both Cr and Au were fixed at either 20 eV , 50 eV , and 100 eV (denoted as D1, D2 and D3 respectively). The range of values chosen for the deposition energy is within the experimental energies typically chosen for deposition of metallic thin films using high-energy deposition processes such as high-energy magnetron sputtering and pulsed laser deposition [46,47]. As the mass of Cr and Au are different, this means that the deposition velocities corresponding to each energy were also different for Cr and Au. All three structures were also annealed at two different temperatures, namely at 700 K and 1000 K , denoted as A1 and A2 respectively. Subsequent results for mechanical and thermal properties will describe the variation of properties of these six structures (D1-A1 to D3-A2).

2.4. Tensile/compression test modelling

Constant strain-rate uniaxial tensile and compressive deformations were applied along the z-direction for the six composite thin film structures [48]. To ensure that the model was well equilibrated, an energy minimization using the conjugate gradient method, followed by equilibration in the isothermal-isobaric ensemble (NPT) were carried out prior to deformation. During tensile or compression deformation, the temperature was fixed under the canonical ensemble, consistent with literature [49]. The entire SiO₂-Cr-Au structure was elongated at a steady strain rate of $0.0001 \text{ \AA/ps}$. Periodic boundary conditions were applied in the z direction to create a bulk-like structure along the z-axis as well, as these composite films are used in sensing and accelerometer applications as one single unit, along with the silica substrate. The resulting stress-strain profiles was used to extract mechanical properties

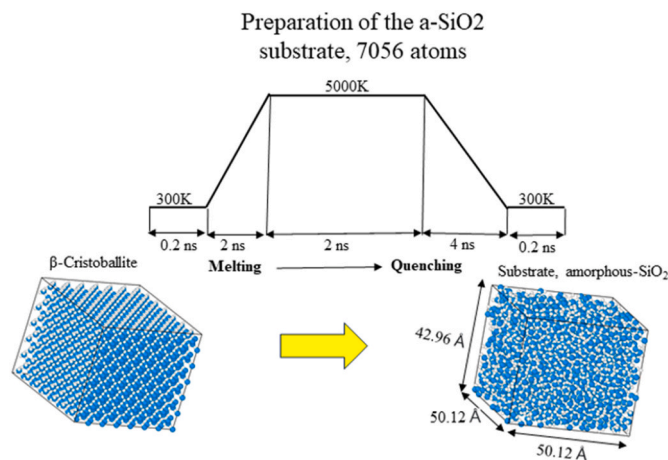


Fig. 2. Preparation of amorphous silica using the melt-quench method. Snapshots of the initial crystalline phase of silica (β -cristobalite) and the final amorphous structure are shown.

as described in section 3.

2.5. Hardness simulations

Atomistic simulations of nanoindentation were performed to calculate the hardness of all the six thin films. A spherical indenter was modelled using a fully repulsive potential, ensuring that no adhesive interaction occurred with the sample surface. After setting the indenter radius at 10 Å, it was pushed into the sample from above the composite film, along the negative z -axis at a steady rate of 0.1 Å/ps. To model a semi-infinite substrate, the bottom atomic layer was fixed, and periodic boundary conditions were added to the lateral directions (x and y). To prevent unphysical reflections and absorb stress waves, a damping layer was added beneath the active deformation zone. Hardness is defined as [50].

$$H = \frac{F_m}{A_p} \quad \text{eq. (i)}$$

where, F_m is the maximum applied force (from the force-displacement curve) and A_p is the projected contact area made by the indenter on the surface at F_m . For the spherical tip, $A_p = \pi(2R^*h_c - h_c^2)$. Here, R denotes the radius of the spherical indenter, set at 10 Å in the simulations, which defines the curvature of the indenter tip and influences the contact geometry. The parameter h_c represents the contact depth, the vertical penetration depth of the indenter into the sample surface at the point of maximum force, accounting for elastic and plastic deformation.

2.6. Coefficient of thermal expansion

The coefficient of thermal expansion (CTE) was calculated for each of the six composite thin film structures over a temperature range from 200 K to 400 K. Simulations were performed at under the NPT ensemble at a temperature range from 200 K to 400 K and at 0 isostatic pressure. From the variation of volume (V) versus temperature (T), quadratic fits [51] of the form $V = a + bT + cT^2$ [2] were applied to extract parameters a , b , and c for each structure and at each temperature. The volumetric thermal expansion coefficient $\beta_v(T)$ was computed using the formula $\beta_v(T) = (b + 2cT)/a$. Here, a is the initial volume at the reference temperature, b represents the linear thermal expansion coefficient, and c accounts for the nonlinear (quadratic) temperature dependence, reflecting anharmonic effects in the lattice. These parameters, extracted from the volume-temperature data, enable a precise characterization of the temperature-dependent thermal expansion behavior, validated against experimental results for metallic thin films. This method ensures an accurate representation of the temperature-dependent behaviour of the material's thermal expansion properties and has shown good agreement with experiments for metallic thin films [51].

3. Results and discussion

3.1. Structural characterisation

The Ackland-Jones analysis [52] is a computational method for identifying local crystal structures in atomic systems by analyzing bond angles between neighboring atoms. Fig. 4 shows the Ackland-Jones analysis for the final composite structure after deposition at three incident deposition energies, depicting structural order for the composite structure. Fig. 4 illustrates the Ackland-Jones analysis of the microstructure evolution in a multi-layered thin film simulated with three different deposition energies – 20 eV, 50 eV and 100 eV. The layers consist of a gold (Au) top layer, a Cr interlayer, and a silicon dioxide (SiO₂) substrate similar to Fig. 3. It is observed that for all three energies, the Cr layer was amorphous and Au formed a polycrystalline (FCC) film comprising stacking faults. The Cr interlayer thickness for the intermediate deposition energy (50 eV), was in between the lowest and highest

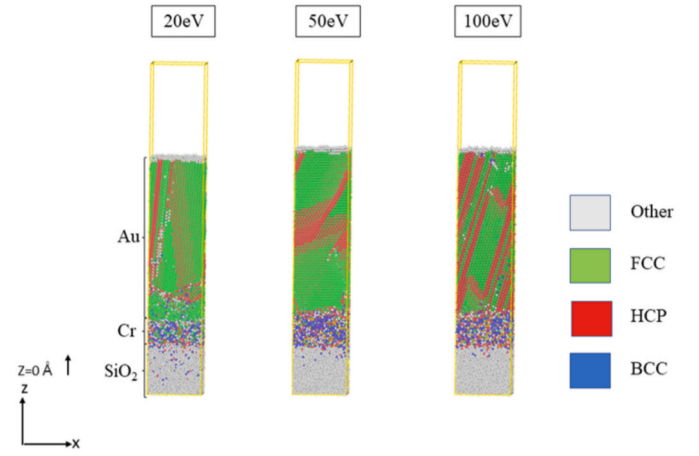


Fig. 4. Atomistic snapshots of the SiO₂-Cr-Au composite structures right after deposition at three different incident energies- 20 eV, 50 eV, 100 eV. Color coding of the atoms are according to the structure determined using the Ackland-Jones Analysis (SiO₂ is amorphous (“other”), Cr is amorphous and Au is polycrystalline, in FCC crystal structure).

energies, with 20 eV yielding a very small interlayer thickness energy. At the highest energy (100 eV), defects in Au, notably stacking faults were enhanced as seen in Fig. 4. Thus, moderate deposition energies lead to the right balance of interlayer thickness and the quality of the Au thin film (in terms of defects). The distribution of phases and the associated dislocation structure emanating in the Au phase at the end of the annealing stage are given in Table 2.

To quantify short range order and coordination of atoms in the thin film, the radial distribution function (RDF) was calculated for all pairs of atomic interactions as shown in Fig. 5 for D1-A1. The inset in the figure shows the coordination number for the interaction types calculated from the integration of the RDF profiles till the end of the first peak. The Si-O $g(r)$ profile matches with published results for amorphous silica [53]. We note that the Cr interlayer is also amorphous owing to the deposition on an amorphous substrate [54]. On the other hand, for all deposited thin films, we observed that Au-Au interactions showed sharp crystalline peaks [55]. The coordination number for both Cr and Au were approximately equal to 12, calculated over the nearest neighbor shell. A very similar $g(r)$ profile was observed for all the six structures reported here.

3.2. Interfacial stresses

To characterize the in-plane stresses developed in the composite films, the longitudinal (zz) and transverse (xy) stress components were calculated as a function of the z -distance, plotted in Fig. 6. The initial large stresses around 0 Å are a consequence of fixing the bottom silica layers as rigid, and are not of any significance. As we move along the z -direction, the first rise in the longitudinal stress occurs at the SiO₂ – Cr interface (dotted black line) owing to the sharp change in interfacial atomic packing. Since the Cr adhesion layer is quite thin, and as a consequence, being amorphous, the interfacial stresses between SiO₂

Table 2

FCC and HCP content and dislocation analysis for the six configurations after annealing.

Configuration	FCC (%)	HCP (%)	Number of Dislocation Lines	Dislocation Length (Å)
D1-A1	42.1	17.7	52	959.268
D1-A2	45.9	12.9	51	893.528
D2-A1	57.7	5.1	0	0
D2-A2	51.7	9.5	11	284.576
D3-A1	30.9	30.7	20	791.824
D3-A2	35.7	24.6	24	727.814

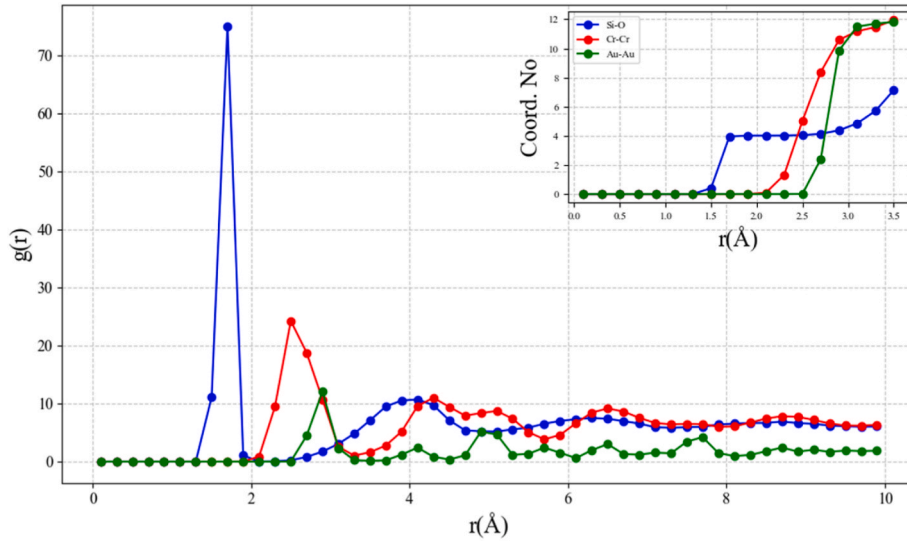


Fig. 5. Radial Distribution Function (RDF) and Coordination Number for different atom pairs (Si-O in blue, Cr-Cr in red, Au-Au in green). The main plot displays $g(r)$, showing the distribution of distances between pairs of atoms (Si-O, Cr-Cr, Au-Au), with peaks indicating preferred nearest neighbor distances. The inset plot shows the cumulative coordination number, providing an integrated measure of atomic neighbors as a function of separation.

and Cr are quite large (of the order of 20 GPa). The large stresses emanate from disparate thermal expansion coefficients and probable compound formation and are difficult to remove by annealing. The stresses reach a value close to 20 GPa, which is similar to those observed for metallic heterostructure metallic thin films that are known to be around 20 GPa [56,57]. Interestingly, we observe only a marginal drop in the as-deposited stresses after annealing (as seen in Fig. 6a) for each of the six structures.

It was also observed that for the higher annealing temperature (A2, 1000 K), there is a tendency for Cr to diffuse into the silica layer (see panels D1-A2 and D3-A2), which leads to a shift in the silica-Cr interface, and correspondingly, the stress values as well. On the other hand, the Cr-Au interface is seen to have an excellent interfacial bonding, leading to close to 0 stress at the interface. The transverse stress component (τ_{xy}), on the other hand oscillates around 0 for all the six structures and does not play a role in the mechanical behavior of the composite film.

3.3. Tensile properties

Uniaxial tensile deformation for the six composite thin film samples were performed as described in section 2.4. The stress-strain curves for the structures are shown in Fig. 7. All structures demonstrate an initial elastic region, followed by the first instance of yielding (that is accompanied by a stress drop), and subsequent strain hardening accompanied by plastic deformation. In the latter stage of plastic strain, a typical saw-tooth like behavior is observed owing to repeated localized yielding and hardening effects [58]. Mechanical properties extracted from the stress-strain curves, such as the Young's modulus, yield point, yield strength, ultimate tensile strength (UTS), strain to failure and toughness are tabulated in Table 3. To measure the statistical significance of the data, three independent simulations arising from independent deposition and annealing stages with different random seeds are reported for the D2-A1 structure. As seen from Fig. 7, the precise processing condition has a huge impact on the final mechanical properties, with both the deposition energy and annealing temperature playing important roles. The maximum Young's modulus, ~ 130 – 140 GPa was observed for the thin films deposited with the intermediate energy (D2; 50 eV). This is also crucial for enhanced yield strength and UTS; however, the maximum toughness and strain to failure were observed for the lowest deposition energy and annealing temperature (D1-A1). For either the lower (D1) or higher (D3) energy, the modulus and strength are reduced

indicating the effect of atomic packing on the tensile properties. An increase in the annealing temperature also led to better mechanical properties in general, but an optimum value of the annealing temperature may need to be ascertained on a case-by-case basis for a composite film for a simultaneous enhancement in all the properties listed above.

The superior mechanical properties of the D2-A1 configuration (Young's modulus: 129.24 GPa, yield strength: 5.01 GPa) correlate directly with its highest FCC content (57.7 %) (see Table 2) and the absence of dislocations, which aligns with fundamental research on crystal structure-property relationships. Research by Guo and Wang [59] on FCC, BCC, and HCP crystal structures demonstrates that FCC structures exhibit superior elastic properties due to their higher atomic packing density and more favorable slip systems compared to HCP structures [60]. The calculated elastic constants show that FCC crystals are inherently more stable against shear deformation, which explains why the D2-A1 configuration with maximum FCC content exhibits the highest Young's modulus. However, though the dislocation-free structure leads to an enhancement in the mechanical properties, the higher annealing temperature may negate this effect more drastically than at other deposition conditions (i.e., those that possess a larger dislocation density prior to deformation). This is supported by the recent work by Chu et al. [25] who showed experimentally that the annealing temperature can lead to non-trivial strengthening effect in SiO_2 -Cr-Au thin films owing to enhanced diffusion of Cr, especially at high annealing temperatures.

The role of dislocations in determining mechanical behavior is well established. Davoudi et al. showed that the dislocation density in metallic thin films directly correlates with stress concentration and reduced mechanical performance [61]. Their research shows that dislocation climb and glide mechanisms lower the overall stress level in thin films and reduce work hardening rates. This explains why configurations D1-A1 and D1-A2, with their high dislocation densities (52 and 51 dislocation lines respectively), exhibit lower yield strengths (2.97 and 2.38 GPa) despite having moderate FCC content. The dislocation-free D2-A1 configuration achieves optimal mechanical properties by eliminating these stress concentration sites.

The processing parameter effects observed in the data are supported by molecular dynamics research on bimetallic systems. Studies on Fe/Cu bimetallic interfaces by Zhang et al. demonstrate that moderate deposition energies promote favorable atomic arrangements while avoiding excessive defect formation [62]. The optimal performance of the 50 eV

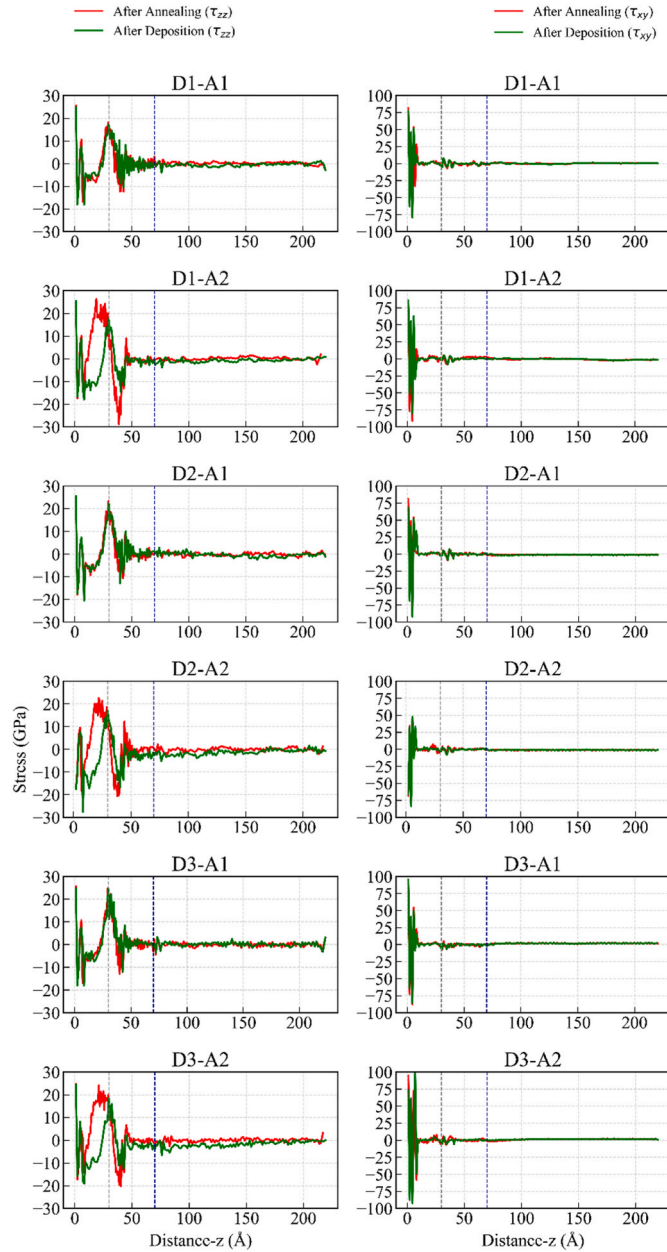


Fig. 6. Stress distribution analysis for the six configurations (D1-A1, D1-A2, D2-A1, D2-A2, D3-A1, and D3-A2) along the deposition (z) axis, comparing stress profiles after deposition (green) and after annealing (red). Longitudinal (τ_{zz}) and transverse stress (τ_{xy}) components are shown in the left and right set of panels respectively. Each configuration exhibits pronounced longitudinal stress peaks and small oscillations for the transverse stress near the silica-Cr interface which gradually diminishes as the distance increases. The dotted black line represents the SiO_2 -Cr interface, and the dotted blue line represents the Cr-Au interface.

deposition energy (D2) compared to lower or higher energies reflects this balance. Additionally, research on Ti/Cu bimetallic systems shows that elevated annealing temperatures (above 800 °C) cause structural degradation and mechanical property reduction [63], which explains why the A2 (1000 K) annealing consistently produces inferior properties compared to A1 (700 K) annealing across all deposition energies.

The stress relaxation mechanisms in thin films, as described by Dong et al.'s molecular dynamics simulations, provide insight into the dislocation formation patterns [64]. Their research demonstrates that compressive misfit strains lead to dislocation nucleation at surface depressions through atomic buckling mechanisms, while tensile conditions

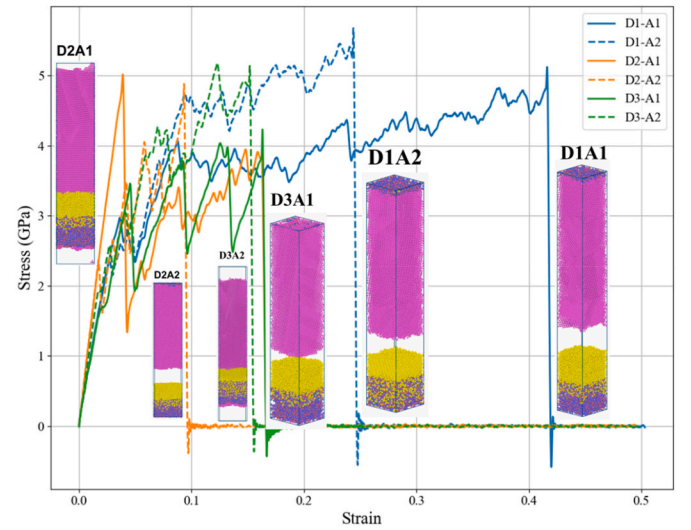


Fig. 7. Stress-strain curves from the tensile deformation of the six SiO_2 -Cr-Au composite films.

promote different nucleation pathways. This mechanistic understanding explains why certain processing conditions (D2-A1) can achieve dislocation-free structures while others inherently generate high dislocation densities, directly impacting the mechanical properties observed in the tensile behavior.

3.4. Compressive properties

The stress-strain curves during compressive deformation for the six films are presented in Fig. 8. Owing to the heterogeneous film and the polycrystalline nature of the gold layer, multiple yielding events are observed, leading to a repetitive saw-tooth like stress-strain profile. The point of the first yield event is seen to be highly dependent on the processing condition of the film, both in terms of the deposition energy and the annealing temperature. The mechanical properties under compression, including the yield stress and strain (at the point of the first yield phenomenon) and the compressive modulus are tabulated in Table 4. As was observed for the tensile properties, we observe that intermediate deposition energy (50 eV) and lower annealing temperature (700 K) yield optimum compressive properties (in terms of larger modulus and limit of yield). An increase in the annealing temperature leads to a marginal reduction in the yield stress and modulus. It is to be noted that the highest deposition energy (100 eV) leads to a drastic decrease in the yield stress, akin to the tensile behavior.

3.5. Hardness

Nanoindentation simulations were performed as described in section 2.5 to ascertain the hardness of the thin films. The samples' significant differences in force–depth response demonstrated how microstructural variations affect mechanical characteristics, as shown in Fig. 9. Compared to their respective D1-A2, D2-A2, and D3-A2 counterparts (i. e. larger annealing temperature of 1000 K), samples D1-A1, D2-A1, and D3-A1 showed larger elastic areas and greater peak forces. This suggests that samples with smaller annealing temperatures generally enhance toughness and are more resilient to plastic deformation. Moreover, differences in the unloading segments suggest variations in the elastic recovery behavior among the different sample types.

The hardness of the films extracted according to eq. (i) is tabulated in Table 5. As observed for tensile properties, intermediate deposition energy (D2, 50 eV) was seen to yield the highest hardness of about 18 GPa (for an annealing temperature of 700 K). For lower and higher deposition energies, the hardness decreases. With the exception of the

Table 3

Mechanical properties estimated from tensile deformation simulations for the six configurations. Data for the D2-A1 configuration has been averaged over three independent structures.

Configuration Name		Young's Modulus (GPa)	Yield Strength (GPa)	Ultimate Tensile Strength (UTS) (GPa)	Fracture Point		Toughness (GPa)
Deposition Energy (eV)	Annealing Temperature (K)				Stress (GPa)	Strain	
D1 (20 eV)	A1 (700 K)	84.17	2.97	5.11	5.11	0.42	1.57
	A2 (1000 K)	89.16	2.38	5.67	5.67	0.24	0.99
D2 (50 eV)	A1 (700 K)	128.26 $\pm$ 0.89	5.09 $\pm$ 0.07	5.16 $\pm$ 0.13	4.44 $\pm$ 0.43	0.20 $\pm$ 0.03	0.64 $\pm$ 0.14
	A2 (1000 K)	140.25	2.36	4.87	4.87	0.09	0.27
D3 (100 eV)	A1 (700 K)	89.16	1.67	4.22	4.22	0.16	0.45
	A2 (1000 K)	114.42	1.92	5.17	5.17	0.15	0.53

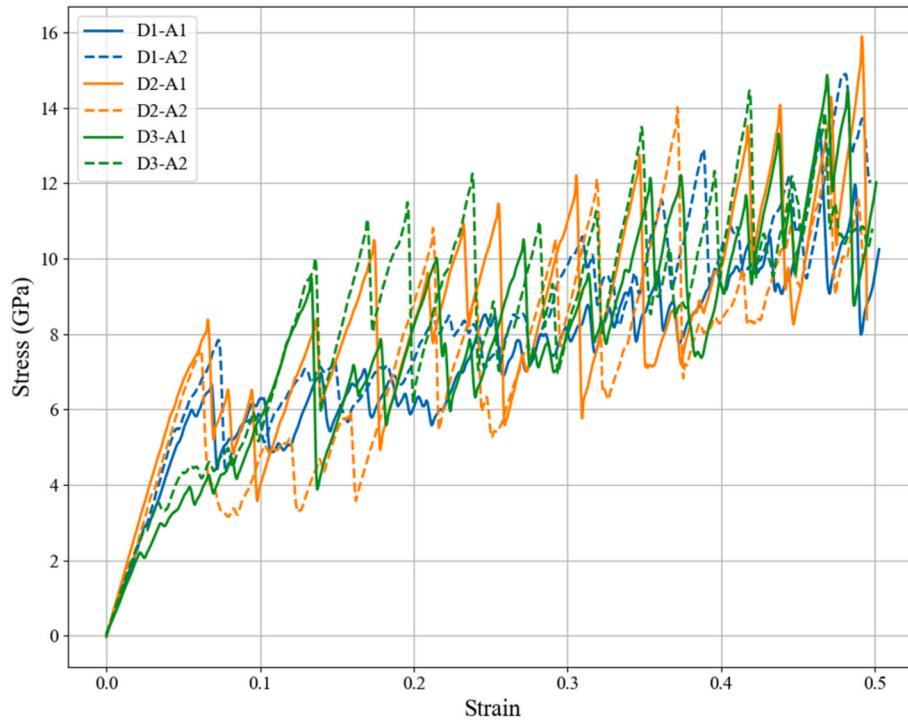


Fig. 8. Compressive modulus for 6 configurations D1-A1, D1-A2, D2-A1, D2-A2, D3-A1, D3-A2.

Table 4

Compression test data calculated using molecular dynamics simulations for 6 configurations. Data for the D2-A1 configuration has been averaged over three independent structures.

Configuration Name		Yield Stress (GPa)	Yield Strain	Modulus (GPa)
Deposition Energy (eV)	Annealing Temperature (K)			
D1 (20 eV)	A1 (700 K)	6.0352	0.05	120.704
	A2 (1000 K)	8.0739	0.078	103.511
D2 (50 eV)	A1 (700 K)	8.56 $\pm$ 0.04	0.073 $\pm$ 0.002	115.72 $\pm$ 2.11
	A2 (1000 K)	7.5595	0.075	100.78
D3 (100 eV)	A1 (700 K)	2.2292	0.02	111.45
	A2 (1000 K)	3.578	0.036	99.388

20 eV (D1) films, an increase in annealing temperature led to a decrease in the hardness which could be due to relieving of the internal stresses that oppose the indentation stress.

We note that our calculated values for mechanical properties can be compared with the recent experimental investigation of SiO₂-Cr-Au composite film by Chu et al. [25] They reported values of 80–107 GPa for the Young's modulus and a hardness of 3.2–4 GPa at annealing

temperatures ranging from 0 to 600 °C.

3.6. Coefficient of thermal expansion

Fig. 10 shows the volumetric CTE values for all six structures calculated at a temperature range of 200–400 K. Overall, no direct temperature-dependence of CTE was observed, with values ranging from 2.5 to 4.5 $\times 10^{-5}$ K⁻¹. These values are low enough for the application of these composite films in sensor and accelerometer applications where minimum thermal expansion is desirable, and are comparable with the CTE of metals like Al (2.2 $\times 10^{-5}$ K⁻¹) and Ti (1 $\times 10^{-5}$ K⁻¹) [65]. In general, a larger deposition energy and a larger annealing temperature lead to a smaller CTE, albeit the difference being only marginal. Increased deposition energy (D3; 100 eV) shows lower thermal expansion in comparison to lower deposition energies.

4. Conclusion

Deposition of SiO₂-Cr-Au composite thin films, which are crucial components in sensors for navigation systems, were simulated using molecular dynamics. Six different processing conditions were employed (three deposition energies and two annealing temperatures) to ascertain

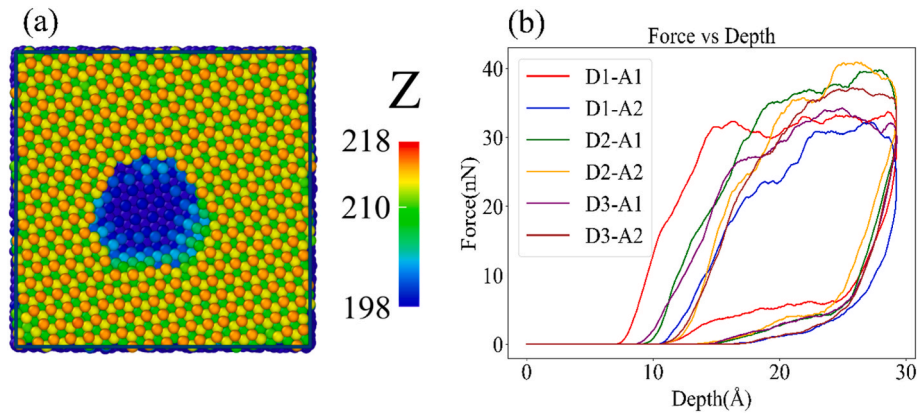


Fig. 9. (a) Top view of the indentation on thin film from above the surface of Au. The blue region shows the indentation from the spherical indenter. The colour code is such that atoms are colored according to their z positions from the top of the surface (218 Å; orange atoms) to the bottom of the indenter (198 Å; blue atoms) in the system. (b) Force vs Depth curves for the six thin film configurations under nanoindentation.

Table 5

Hardness for the six structures calculated from MD simulations. Data for the D2-A1 configuration has been averaged over three independent structures.

Configuration	Hardness (GPa)
D1-A1	5.37
D1-A2	8.30
D2-A1	15.29 ± 2.52
D2-A2	12.06
D3-A1	9.15
D3-A2	6.06

the relationship between processing, structure and properties of the thin films. Since the Cr adhesion layer is quite thin, and as a consequence, being amorphous, the interfacial stresses between SiO₂ and Cr are quite large (of the order of 20 GPa). The large stresses emanate from disparate thermal expansion coefficients and probable compound formation and are difficult to remove by annealing. An increase in deposition energy initially enhances Young's modulus and yield strength followed by a subsequent reduction in mechanical properties under tensile deformation. Similarly, greater annealing temperatures (1000 K) increase stiffness but generally diminish yield strength, demonstrating a delicate balance between elasticity and strength. Under compressive loading, the maximum yield stress was observed for intermediate deposition energy

and lower annealing temperature, followed by a drastic reduction in yield stress for larger deposition energy.

The hardness of films also shows a similar trend in that intermediate deposition energies and lower annealing temperatures are beneficial for enhancement in properties. Coefficient of thermal expansion was calculated for the films, and it ranges from 2.5 to $4.5 \times 10^{-5} \text{ K}^{-1}$, suitable for applications that require structural integrity and low thermal expansion. It was observed that the processing conditions have a non-trivial and marginal effect on thermal expansion. Ultimately, the processing-structure-properties relations developed here can help in designing next-generation electronic devices by providing valuable insights for the design and manufacturing of thin-film systems employed in sensors and accelerometers that are more dependable and efficient.

CRediT authorship contribution statement

Tejasva Vashistha: Writing – original draft, Visualization, Validation, Software, Investigation, Formal analysis, Conceptualization, Methodology, Data curation. **Kishalay Raj:** Visualization, Investigation, Formal analysis, Data curation. **Harshit Kumar Gupta:** Writing – review & editing, Validation, Resources, Methodology, Conceptualization. **Raghavan Ranganathan:** Writing – review & editing, Validation, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization.

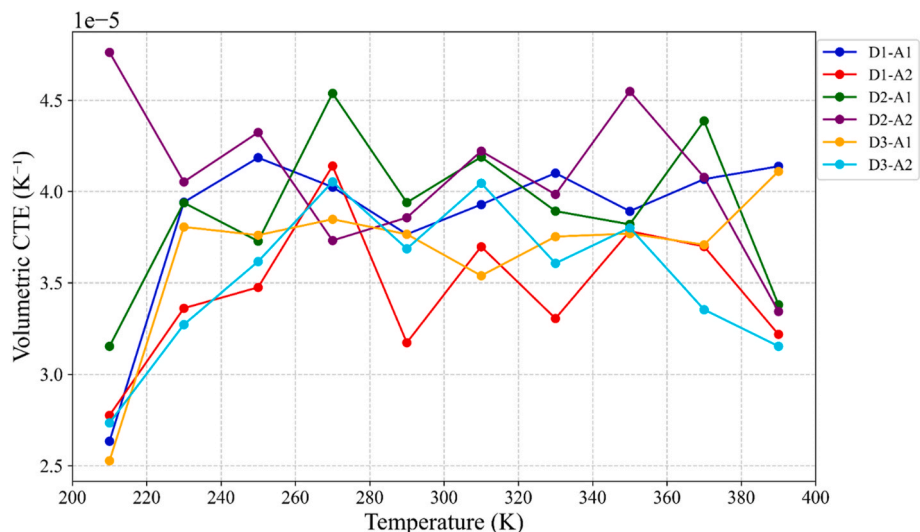


Fig. 10. Volumetric coefficient of thermal expansion, $\beta_v(T)$ as a function of temperature for the six thin film composite structures.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Raghavan Ranganathan reports financial support was provided by Indian Space Research Organization. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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