

Multicomponent intermetallic nanoparticles and superb mechanical behaviors of complex alloys

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Relevance to the group

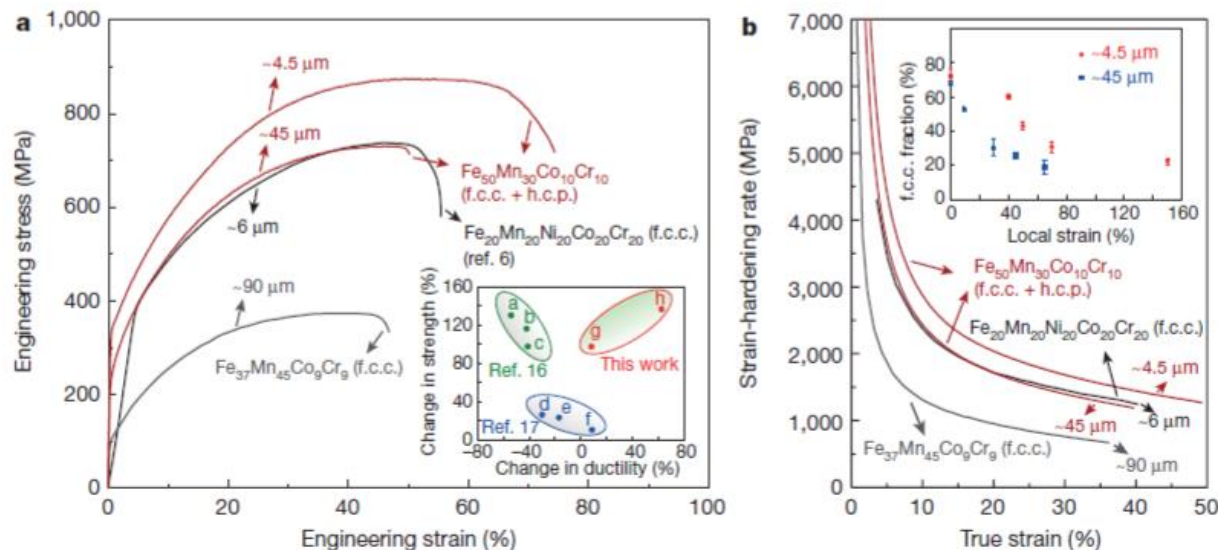
- We are trying to synthesise high entropy alloys using ambient electrospray technique.
- Characterization technique, property studies may help us.

In this paper

- They developed an innovative design strategy to eliminate ductility loss in gigapascal-strength alloys.
- This design concept aims to controllably create the ductile multicomponent intermetallic nanoparticles (MCINPs) for coherent strengthening in the fcc-type HEA systems.
- They have achieved in situ ductilization with a nanoscale precipitation of MCINPs by controlling the order-disorder phase transformation and elemental partition.
- Two model alloys, $(\text{FeCoNi})_{86}\text{-Al}_7\text{Ti}_7$ (**Al₇Ti₇**) and $(\text{FeCoNi})_{86}\text{-Al}_8\text{Ti}_6$ (**Al₈Ti₆**), to illustrate the proof of concept based on systematic thermodynamic calculations, by highly alloying with Ti and Al additions, they successfully introduced high-density L1_2 intermetallic nanoparticles in the FeCoNi-base alloy systems.
- Here they selected the FeCoNi for the matrix to achieve a large “FCC+ L1_2 ” dual-phase region for a dense precipitation.
- The partial partitioning of Fe and Co atoms into the L1_2 phase helped to improve the intrinsic ductility of the L1_2 intermetallic phase.

Metastable high-entropy dual-phase alloys overcome the strength–ductility trade-off

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Conceptual design and microstructural characterizations of the MCINPS alloys

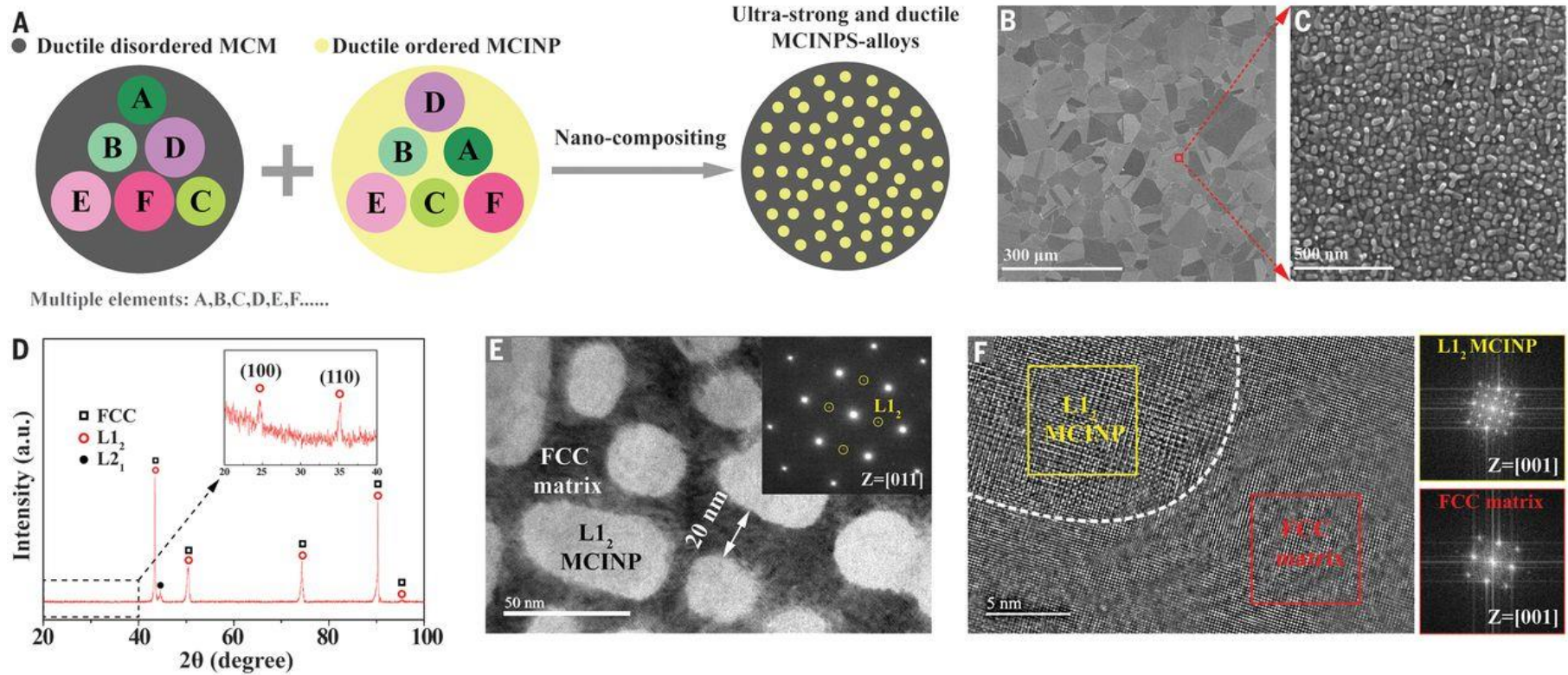


Fig. 1. Conceptual design and microstructural characterizations of the MCINPS alloys. (A) Schematic of the design concept of the MCINPS alloys. MCM, multicomponent matrix. (B) Scanning electron microscopy (SEM) image of the Al_7Ti_7 alloy exhibiting the typical equiaxed grain structures. (C) SEM image of the Al_7Ti_7 alloy revealing the uniform distribution of high-density $L1_2$ MCINP within the grain interior. (D) XRD patterns showing the phase compositions of the Al_7Ti_7 alloy. a.u., arbitrary units. (E) TEM image of the Al_7Ti_7 alloy showing the nanostructured morphology. The inset shows the corresponding SAED pattern. (F) Representative high-resolution TEM image confirming the interfacial coherency.

Spatial morphology and multicomponent nature of the MCINPs

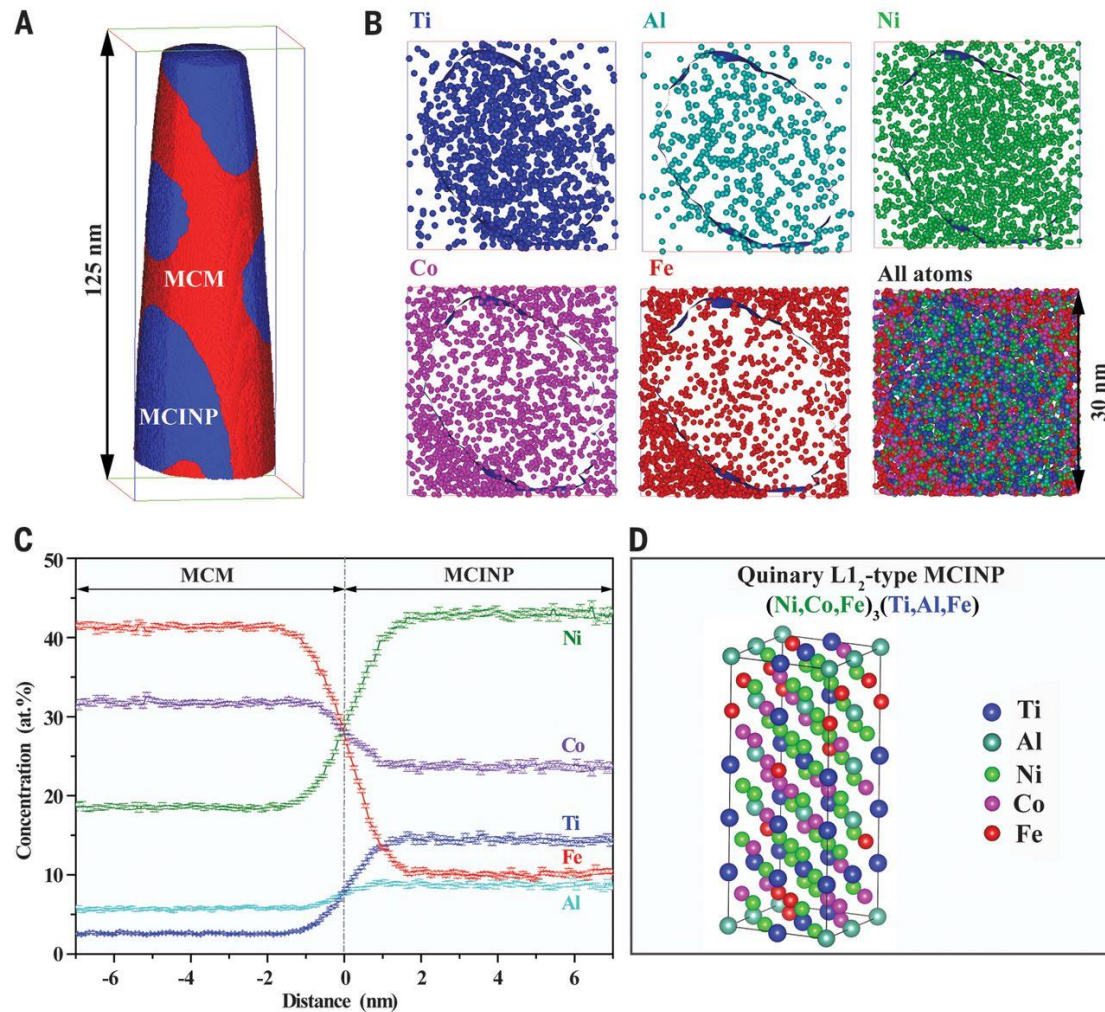


Fig. 2. Spatial morphology and multicomponent nature of the MCINPs.

(A) 3D reconstruction map of an APT needle tip confirming the nanocomposited microstructure of the Al₇Ti₇ alloy.

(B) High-resolution atom maps showing the atomistic distribution within the L1₂ MCINP of the Al₇Ti₇ alloy. (C) Proximity histogram across the matrix and nanoparticles revealing the multicomponent nature of the MCINPs of the Al₇Ti₇ alloy.

(D) Ordering crystallographic structure and site occupancy of the L1₂ MCINP by density functional theory (DFT) calculations of the Al₇Ti₇ alloy.

Compositional analysis

Table S1.

Chemical compositions (at. %) of the newly designed MCINPS-alloys predicted by the thermodynamic calculations at 780 °C.

Alloys	Phases	Composition (at. %)				
		Fe	Co	Ni	Al	Ti
Al7Ti7	Overall	28.67	28.67	28.67	7	7
	L1 ₂	6.7	21.3	47.0	11.4	13.4
Al8Ti6	Overall	28.67	28.67	28.67	8	6
	L1 ₂	6.7	21.1	47.3	12.9	12.0

DFT calculation for structural analysis

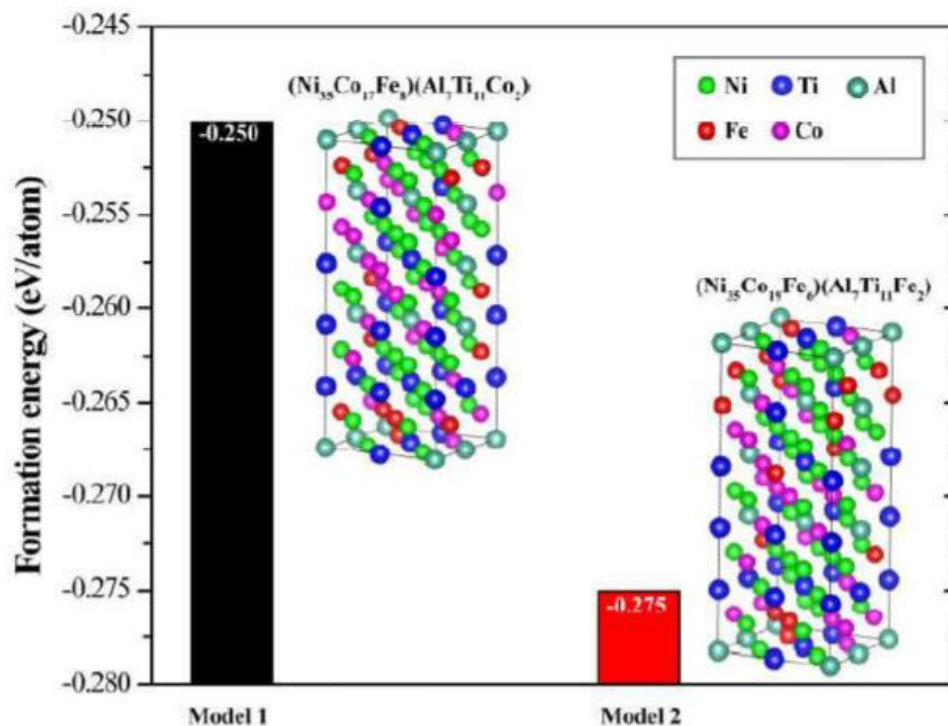


Fig. S7.

DFT calculations of formation energies of the complex A_3B -type MCINP with different sublattice occupancies.

Exceptional strength-ductility combination achieved in the MCINPS alloys at ambient temperature.

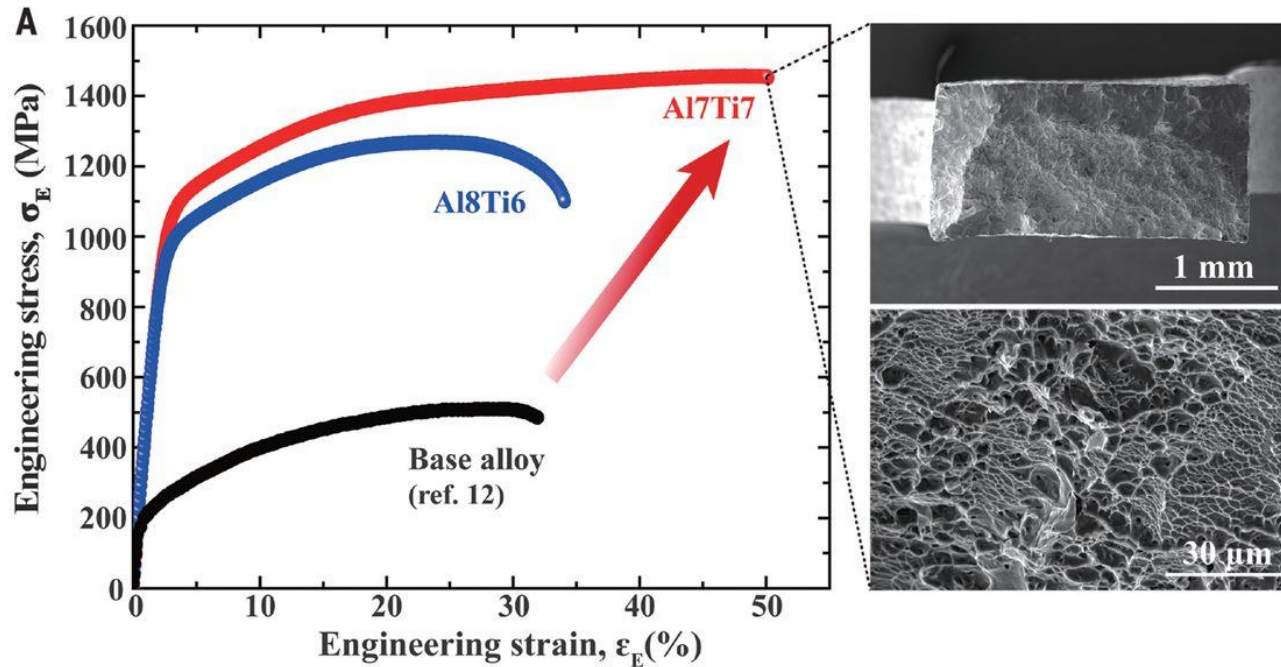


Fig. 3. Exceptional strength-ductility combination achieved in the MCINPS alloys at ambient temperature. (A) Engineering stress-strain curves of the MCINPS alloys compared with the FeCoNi base alloy (12), showing a significant increase of strength without ductility reduction. The Al₇Ti₇ alloy exhibits ductile dimpled structures without macroscopic necking.

Multistage work-hardening behaviours and deformation micro mechanisms of the MCINPS alloys at ambient temperature.

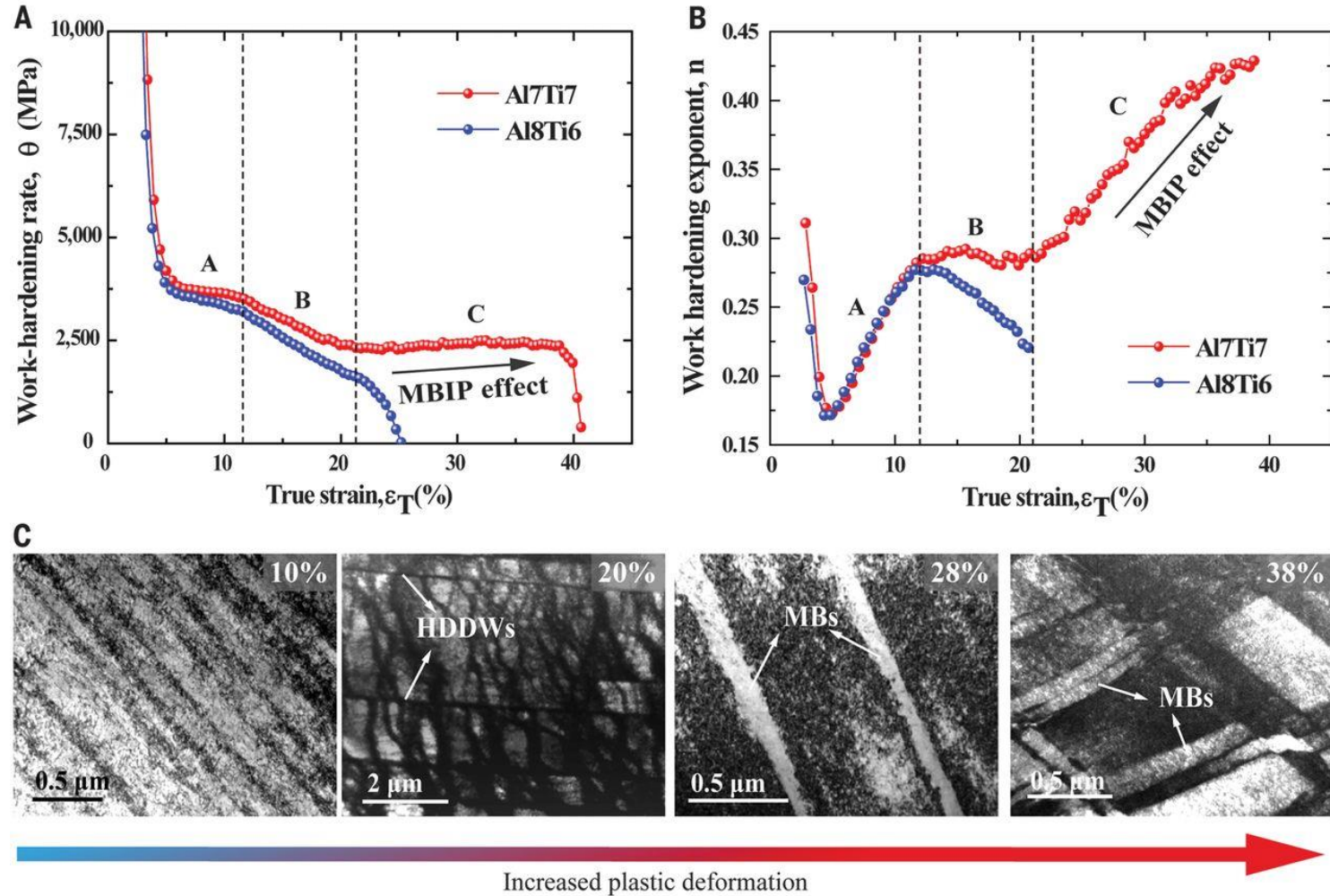


Fig. 4. (A) Work hardening rate curves of the MCINPS alloys. (B) Dynamic change of the work-hardening exponent (i.e., the instantaneous work hardening exponent) within the uniform deformation process of the MCINPS alloys. (C) Dynamic evolution the deformation substructures of the Al₇Ti₇ alloy with increasing tensile loading.

Conclusion

- They proposed an innovative alloy design strategy by engineering high-density MCINPs in complex alloy systems to achieve superb mechanical properties at ambient temperature.
- They demonstrated experimentally that the MCINPS alloys are simultaneously ultrastrong and ductile, with no strength-ductility trade-off and plastic instability.
- This alloy design strategy can also be feasibly applied to many other alloy systems, such as nanostructured alloys, steels, superalloys, and also HEAs, to achieve desired and enhanced properties for specific applications.
- The resulting new-generation complex alloys could lead to superior structural properties, which are of both great fundamental and applied importance for advanced engineering applications involving automobiles, bullet trains, cryogenic devices, and aircraft and aeronautic systems

Thank you