The Influence Mechanism of CSH-Montmorillonite Interface Characteristics on Strength Properties of Cement-Stabilized Montmorillonite

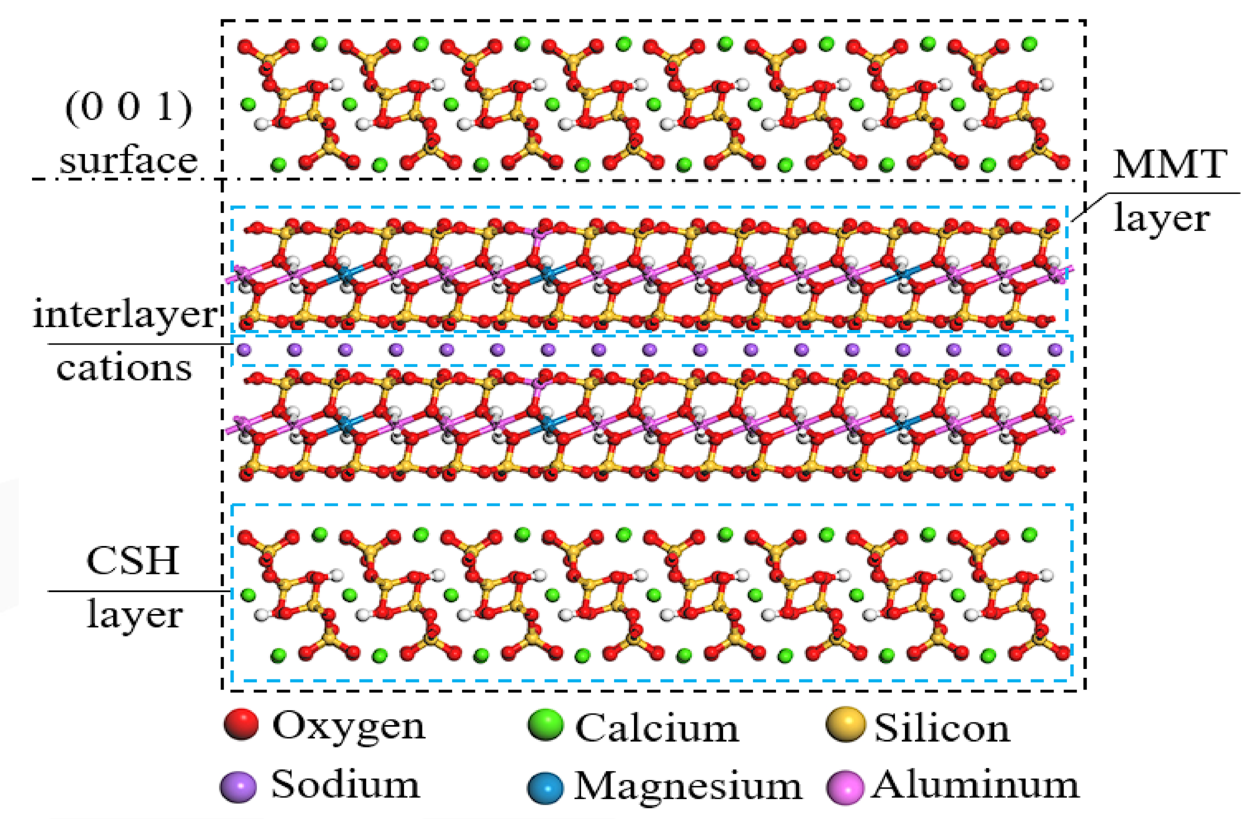
Ge Jinyu[1]；Wang Qiang[2]；Peng Hu[2]； Zhou Juan[2]；Xu Fei[1]；Qian Wenxun[1]
1.Nanjing Hydraulic Research Institute；2. Nanjing Highway Development Center

Objectives

Cement-stabilized soil (cemented soil) technology is an important technical means to improve the poor soil properties such as mucky clay. The existing research on the development mechanism of cemented soil performance is mostly focused on the hydration of cement to characterize the products and microstructures. However, there is still a lack of analysis of the nanoscale interface bonding mechanism between hydration products and clay minerals in cemented soil and the interface energy source of cemented soil. Molecular Dynamics (MD) method can effectively explain the interactions and energy variations between different phases from the nanoscale. However, due to the need to consider the role of clay minerals, model construction and verification are more complicated. The current research focuses on the mechanical and structural evolution of a single material under different variables. There is little analysis of the dynamic mechanism of the interaction between cement hydration products and soil mineral interface areas in cemented soil, and the mechanism of performance improvement of cemented soil has not been fully elucidated.

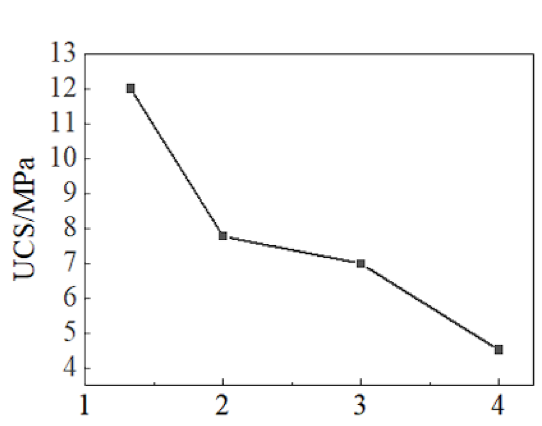
Methods

- **The unconfined compressive strength (UCS) test** was used to explore the effects of different water-to-cement ratio and cement-to-soil ratio on the macroscopic mechanical properties of cement-stabilized Montmorillonite.
- **The Molecular Dynamics (MD) method** was used to quantitatively calculate the energy of the interface area between montmorillonite and CSH.
- **Grey relational analysis** and **X-ray diffraction (XRD)** were used to explore correctness and deviation source of MD model.

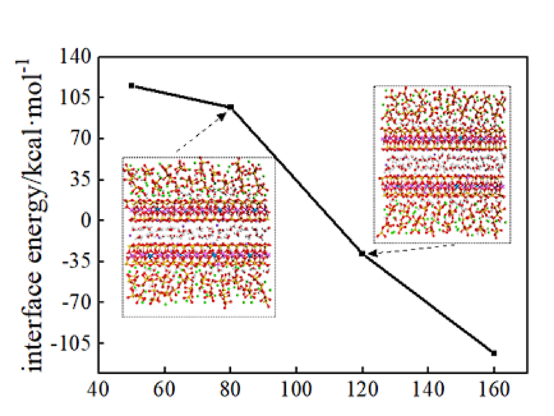


Results

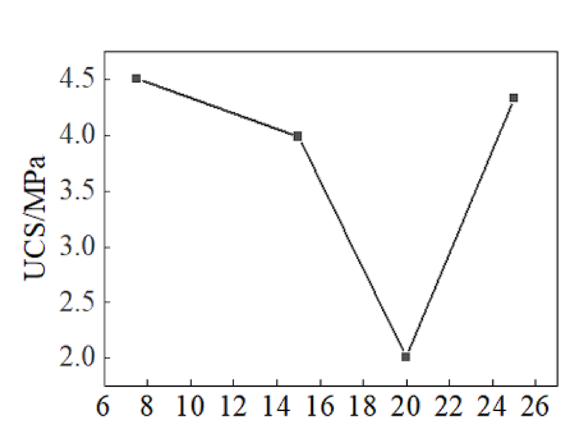
Using grey relational analysis, we find that UCS has a good correlation with CSH-montmorillonite interface energy. The reason is that when the interface energy is high repulsive, the CSH-montmorillonite interface inhibits the dispersion of montmorillonite, resulting in higher stability of the system, which shows better mechanical properties, and vice versa.



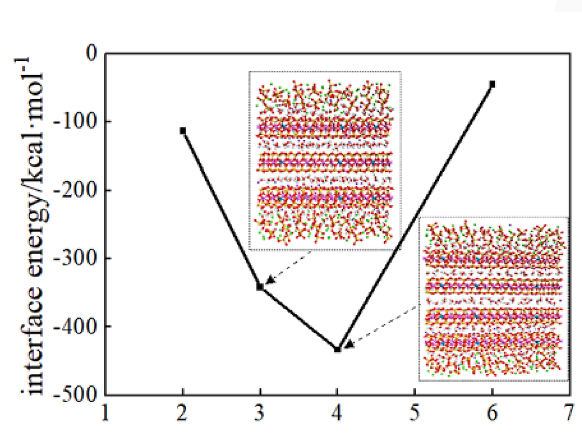
Effect of water-to-cement ratio on UCS



Effect of water molecule number on interface energy



Effect of cement-to-soil ratio on UCS



Effect of MMT layers number on interface energy

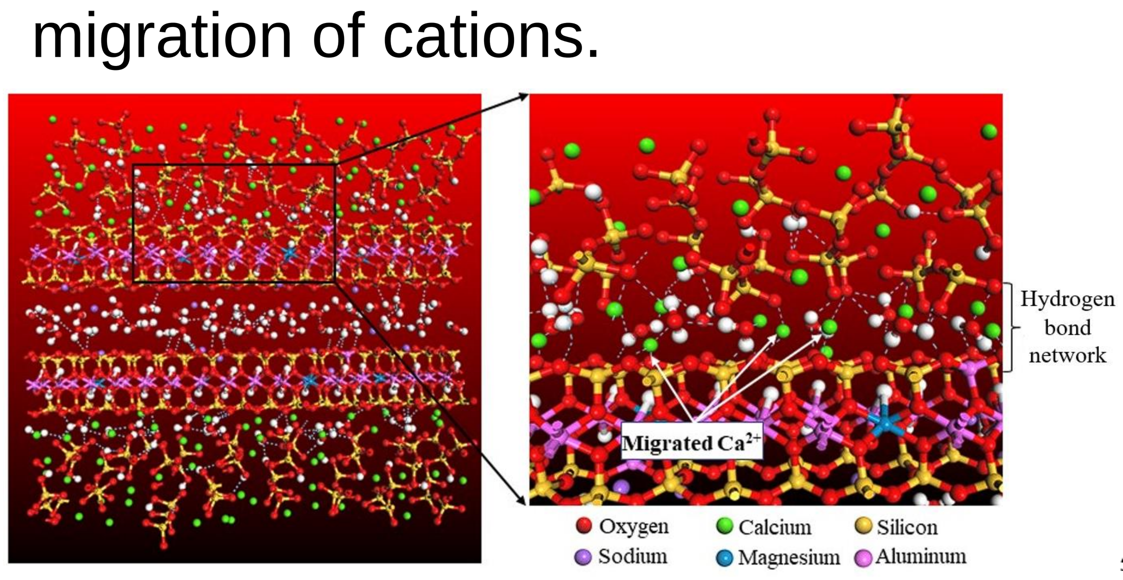
Correlation coefficient under the same cement-to-soil ratio and different water-to-cement ratio

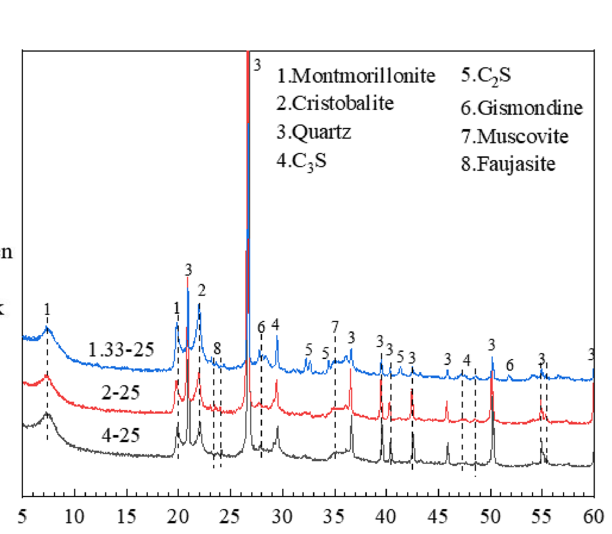
Water-to-cement ratio	1.33	2	3	4	Grey correlation degree
ξ_0	1	0.85	0.33	1	0.80

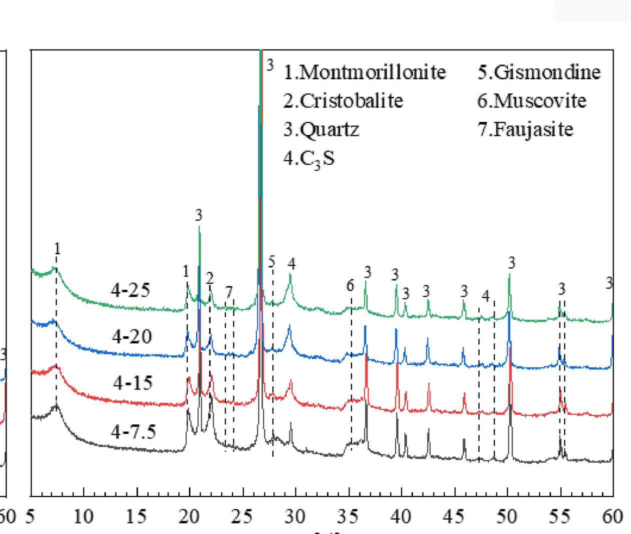
Correlation coefficient under the different water-to-cement ratio and same cement-to-soil ratio

Cement-to-soil ratio/%	7.5	15	20	25	Grey correlation degree
ξ_0	0.61	0.33	1	0.79	0.69

Using the MD method, we find that the CSH-montmorillonite interface energy is mainly composed of van der Waals energy, hydrogen bond energy and electrostatic energy, and their lines and electrical properties are caused by the migration of cations.







Using XRD test, we find that the migration characteristics of Ca^{2+} and Na^{+} are consistent with the results of MD simulation, which proves the correctness of MD model.

Conclusions

- The CSH-montmorillonite interface energy consists of van der Waals energy, hydrogen bond energy and electrostatic energy.
- CSH-montmorillonite interface energy has good agreement with the UCS of the cemented soil, the interface energy decreases with increasing number of water molecules and decreases then increases with increasing number of layers of montmorillonite.
- The repulsive force at the CSH-montmorillonite interface can be maximized or the gravitational force minimized by adjusting the water-to-cement ratio and the cement-to-soil ratio, thus controlling the strength performance of the cemented soil to optimize it.
- XRD analysis results reflect that the migration characteristics of Ca^{2+} and Na^{+} under different water-to-cement ratio and cement-to-soil ratio are consistent with the MD simulation results.

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