

## Constraints

The inequality constraints defining the feasible space among  $C_{11}$ ,  $C_{22}$ , and  $C_{12}$ , along with one equality constraint representing the linear relation between  $C_{12}$  and  $C_{66}$ , are shown in Equations (S-1) and (S-2), respectively, with all values expressed in ‘GPa’. The numerical coefficients presented in Equation (S-1) are derived from the property closure of IN-718 alloy following the four-step procedure described in section II. Additionally, the surfaces corresponding to all inequality constraints are illustrated in cyan color in Fig. 1.

$$\left. \begin{aligned}
 &0.27685C_{11} + 0.27685C_{22} + 0.92017C_{12} \leq 270.44284 \\
 &-0.15576C_{11} - 0.15066C_{22} + 0.97624C_{12} \leq 47.22389 \\
 &-0.63256C_{11} - 0.05766C_{22} - 0.77236C_{12} \leq -278.51010 \\
 &-0.64474C_{11} + 0.40416C_{22} - 0.64882C_{12} \leq -134.13403 \\
 &0.32903C_{11} + 0.80507C_{22} - 0.49356C_{12} \leq 285.55942 \\
 &-0.62874C_{11} + 0.45171C_{22} - 0.63297C_{12} \leq -113.88138 \\
 &0.39886C_{11} + 0.51041C_{22} + 0.76184C_{12} \leq 351.93696 \\
 &0.80507C_{11} + 0.32903C_{22} - 0.49356C_{12} \leq 285.55942 \\
 &0.51041C_{11} + 0.39886C_{22} + 0.76184C_{12} \leq 351.93696 \\
 &0.42855C_{11} + 0.42855C_{22} + 0.79541C_{12} \leq 339.95893 \\
 &0.45171C_{11} - 0.62874C_{22} - 0.63297C_{12} \leq -113.88138 \\
 &-0.05766C_{11} - 0.63256C_{22} - 0.77236C_{12} \leq -278.51010 \\
 &-0.15066C_{11} - 0.15576C_{22} + 0.97624C_{12} \leq 47.22389 \\
 &0.27685C_{11} + 0.27685C_{22} + 0.92017C_{12} \leq 270.44284 \\
 &0.40416C_{11} - 0.64474C_{22} - 0.64882C_{12} \leq -134.13403 \\
 &-0.15321C_{11} - 0.15321C_{22} + 0.97625C_{12} \leq 47.22683
 \end{aligned} \right\} \tag{S-1}$$

$$C_{66} = 1.0018C_{12} - 34.736 \tag{S-2}$$