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岩浆热液矿床成矿过程数值模拟与成矿预测

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摘　要:数值模拟方法为定量解析岩浆热液矿床的成矿过程提供了关键技术手段,对揭示控矿机理与指导成矿预测研究具有重要意义.近年来,伴随计算地球科学的迅速发展,成矿过程数值模拟研究取得了显著进展,在多个层面为成矿预测提供了有力支撑.本文系统梳理了成矿过程数值模拟的基本理论与方法,综合评述了当前数值模拟在刻画成矿过程、解析控矿机理以及支撑成矿预测等方面的研究现状,并对数值模拟方法在未来成矿预测中的发展方向作出展望.未来研究将在力-热-化-流全耦合模拟、高性能数值算法开发以及多元信息智能融合等方面持续深化,共同推动成矿预测向物理机制与数据协同驱动的新范式发展.

关键词:岩浆热液矿床;数值模拟;成矿过程;控矿机理;成矿预测;矿床学.

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Numerical Modeling of Ore-Forming Processes and Mineral Prospectivity Modeling for Magmatic-Hydrothermal Deposits

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Abstract: Numerical modeling provides a key approach for quantitatively analyzing the ore-forming processes, revealing ore location mechanisms, and facilitating mineral prospectivity studies for magmatic-hydrothermal deposits. In recent years, with the rapid advancement of computational geosciences, significant progress has been made in numerical modeling of ore-forming processes, which provides critical support for metallogenic prediction in multiple aspects. We summarize the fundamental theories and methods of numerical modeling, provide a comprehensive review of current research regarding advances in simulating ore-forming processes, analyzing ore location mechanisms, and facilitating metallogenic prediction. Finally, we conclude with an outlook on the future development of numerical modeling in advancing metallogenic prediction. We propose that future research should focus on advancing coupled mechanical-thermal-chemical-fluid processes modeling, developing efficient numerical methods, and promoting the intelligent integration of multi-source data. These efforts will collectively drive

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the evolution of mineral prospectivity modeling toward a new paradigm characterized by mechanism-data synergistic modeling.

Key words: magmatic-hydrothermal deposits; numerical modeling; ore-forming processes; ore location mechanisms; mineral prospectivity modeling; ore deposits.

岩浆热液的成矿过程是由岩浆热液作用驱动下的成矿物质活化、运移、沉淀的高度非线性动力学系统,是化学反应、热传递、流体流动和岩石变形等因素耦合作用的结果(於崇文,1994;Hobbs *et al.*,2000;Cox,2005;翟裕生,2007).成矿过程数值模拟是以数学、物理及化学的基本规律为原理,通过建立表征成矿过程的定量化数学模型(数学物理方程),来描述和分析成矿动力学系统的方法技术,其发展进程从早期单场简化模型为主(White,1971;Norton and Knapp,1977),并随着高性能计算和热液系统中多场耦合关系数学理论的发展(Phillips, 1991; Hobbs *et al.*,2000),逐步建立起三维多场(热-流-力-化)耦合模拟体系(Ord *et al.*,2009;Ord *et al.*,2012).已有研究显示,成矿过程数值模拟方法能够有效地将矿床研究从静态推向动态、从定性转变为定量,从而深化对成矿作用的理解,并推动成矿理论研究的不断深入(Ord and Oliver,1997;赵崇斌等,2008;刘亮明等,2010;Weis *et al.*,2012;袁峰等,2019a;朱静和陈建平,2019;黄沁怡等,2021;陈伟林和肖凡,2023).

成矿预测是综合利用成矿理论和勘查方法实现科学找矿的重要途径,如何以最低成本实现找矿成功率的跃升是成矿预测的核心任务(叶天竺等,2007;赵鹏大,2007).目前,指导成矿预测的理论方法包括矿床成矿系列(系统)理论、“三联式”定量预测理论、非线性成矿预测理论、综合信息矿产预测理论等方法(程裕淇等,1979;赵鹏大,2002;成秋明,2006;王世称等,2010).其中,综合信息矿产预测理论方法由王世称等人于20世纪80年代提出,以反映地质体时空关系的地质信息为先导,通过系统融合地球物理、地球化学、遥感等多元找矿信息构建成矿潜力评价模型,并在机器学习技术的推动下逐步实现从经验驱动向数据驱动的快速发展,为矿产资源勘查评价提供重要支撑(陈永清和王世称,1995;王世称等,1999;左仁广,2021;周永章等,2021;肖克炎等,2023;师路易和左仁广,2026;张明明等,2026).近年来,在找矿工作重心向深部隐伏矿体转移以及三维地质信息技术快速发展的背景下,多种三维成矿预测方法与流程相继涌现,如基于“立方体模型”的区域隐伏矿体三维定量预测评价(陈建平等,2007,2014)、基于三维可视化信息分析技术的大比例尺矿产预测方法(肖克炎等,2012)、“地质信息集成-成矿信息定量提取-立体定量预测”深部矿产资源三维预测方法(毛先成等,2011,2016)、基于综合信息的“四步式”三维成矿预测方法(袁峰等,2014,2018,2019b),目前已成为深部矿产勘查预测的重要技术手段.然而,其效能受限于三维预测信息的稀疏性、不确定性和概念性的成矿理论难以转化为有效的预测数据等多方面因素(袁峰等,2024;毛先成等,2026).

面对上述问题,成矿过程数值模拟方法以传统矿床学理论为基础,通过正演再现成矿动力学过程,在深化成矿理论,定量解析矿床规模、定位空间及矿体形态等控制因素的同时,不仅能够直接指示深部有利靶区,更可为成矿预测方法提供蕴含矿床成因机理的成矿指示信息(Li *et al.*,2019;Liu *et al.*,2022;Xiao *et al.*,2024a).

因此,本文以岩浆热液矿床为研究对象,在梳理成矿过程数值模拟方法的基础上,围绕解析矿床的成矿过程、控矿机理以及支撑成矿预测等方面展开论述,并对成矿过程数值模拟在未来成矿预测中的发展方向作出展望,以期能够进一步促进岩浆热液矿床定量化研究和成矿预测可靠性的发展,为推动成矿预测向“物理机制+数据智能”驱动范式的转变提供基础指导.

1　成矿过程数值模拟方法

成矿过程数值模拟方法应用一系列遵循物理化学规律的偏微分方程组来表征其动力学过程.目前针对岩浆热液矿床成矿过程的数值模拟研究主要涉及形变、流体流动、热传递以及化学反应耦合的多物理化学场模拟(图1),并应用有限元法、有限差分法、格子玻尔兹曼法等数值计算方法求解偏微分方程组.

1.1　形变模拟

岩石在受构造应力和流体压力时会发生弹性变形和塑性屈服.通常,假设岩石由一系列均质微元组成,一般研究过程会从微元颗粒角度在岩石发生弹性变形时应用胡克定律表征,其中应变增量是应力增量的线性函数,适用于层状沉积岩的横观各向同性弹性本构方程被定义为(Hill,1998;王者超等,2018):

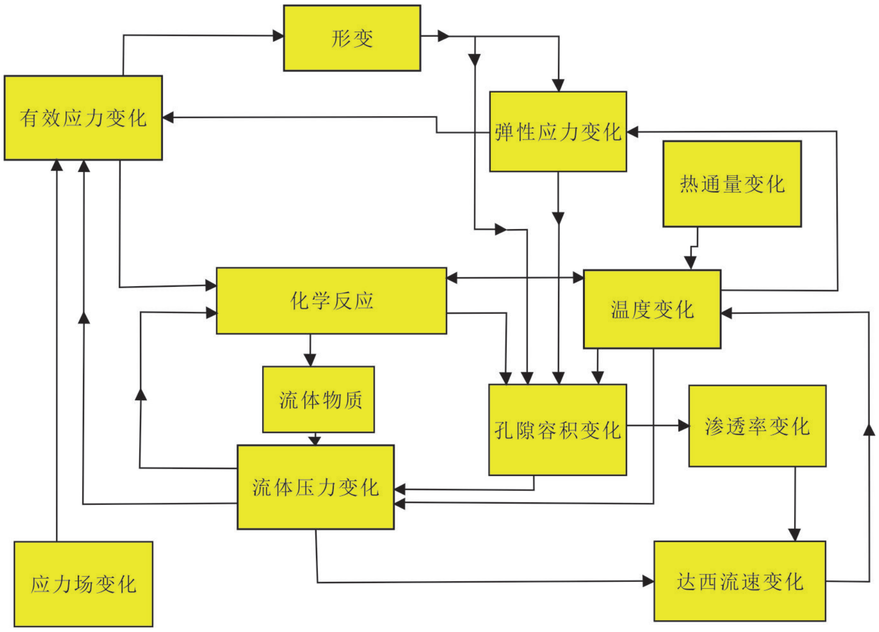

图1 形变-流体流动-热传递-化学反应耦合反馈关系(据Ord *et al.*,2012)

Fig.1 Feedback relations in the fully coupled deformation-fluid flow-thermal transfer-chemical reaction (after Ord *et al.*,2012)

$$\begin{bmatrix}\Delta\varepsilon_x\\ \Delta\varepsilon_y\\ \Delta\varepsilon_z\\ \Delta\gamma_{yz}\\ \Delta\gamma_{zx}\\ \Delta\gamma_{xy}\end{bmatrix}=\begin{bmatrix}\frac{1}{E_{\mathrm{h}}} & -\frac{V_{\mathrm{hh}}}{E_{\mathrm{h}}} & -\frac{V_{\mathrm{vh}}}{E_{\mathrm{v}}} & 0 & 0 & 0\\ -\frac{V_{\mathrm{hh}}}{E_{\mathrm{h}}} & \frac{1}{E_{\mathrm{h}}} & -\frac{V_{\mathrm{vh}}}{E_{\mathrm{v}}} & 0 & 0 & 0\\ -\frac{V_{\mathrm{vh}}}{E_{\mathrm{v}}} & -\frac{V_{\mathrm{vh}}}{E_{\mathrm{v}}} & -\frac{1}{E_{\mathrm{v}}} & 0 & 0 & 0\\ 0 & 0 & 0 & \frac{1}{G_{\mathrm{vh}}} & 0 & 0\\ 0 & 0 & 0 & 0 & \frac{1}{G_{\mathrm{vh}}} & 0\\ 0 & 0 & 0 & 0 & 0 & \frac{2(1+V_{\mathrm{hh}})}{E_{\mathrm{h}}}\end{bmatrix}\begin{bmatrix}\Delta\sigma_x\\ \Delta\sigma_y\\ \Delta\sigma_z\\ \Delta\tau_{yz}\\ \Delta\tau_{zx}\\ \Delta\tau_{xy}\end{bmatrix}, \tag{1}$$

其中,E_{v}(Pa)为垂直于各向同性平面的弹性模量;E_{h}(Pa)为平行于各向同性平面的弹性模量;V_{vh}为施加垂直应变引起水平应变的泊松比,V_{hh}为各向同性平面内的泊松比;G_{vh}(Pa)为垂直于各向同性平面的剪切模量;$\Delta\varepsilon$为应变增量;$\Delta\sigma$(Pa)为正应力增量;$\Delta\gamma$(Pa)为切应变增量,$\Delta\tau$(Pa)为剪切应力增量.

当地质体所受应力达到其屈服强度时,材料行为将由弹性转为塑性,并产生永久变形.应用较为广泛的岩石破裂准则有:屈特加准则、摩尔-库伦准则、格里菲斯准则、最大有效力矩准则等(侯泉林等,2018).岩石屈服准则的适用性强烈依赖于围压条件,需依据具体应力环境进行选择.

由于在成矿过程中岩石受到了温度和流体等因素影响,会发生脆性变形、脆-韧性过渡域变形和塑性蠕变等一系列复杂变形过程,摩尔-库伦准则能够较好地表征临界应力状态下岩石的弹性变形和塑性屈服行为,其线性强度包络线能有效描述大多数岩石在成矿过程围压条件下的力学响应,同时可直接计算出因剪切破坏导致的扩容效应,所以应用较为广泛:

$$\tau=c+\sigma\cdot\tan(\varphi), \tag{2}$$

其中,τ(Pa)为剪切应力,c(Pa)为黏聚力,σ(Pa)为正应力,φ(rad)为内摩擦角.

1.2 流体流动模拟

在成矿过程数值模拟研究中,为刻画热液流体在岩石中的流动行为,通常将岩石概化为多孔介质,从而用达西定律作为其流动控制方程(Chi and Xue,2011).该模型基于如下基本假设:流体在孔隙通道中呈层流状态,同时流体所受惯性力远小于黏滞力,即流线平行、稳定,没有涡旋和混合,且在雷诺数(Re)位于1~10的范围内适用(Manning and Ingebritsen,1999;Cox,2005).在此框架下,将多孔介质中的流体达西速度定义为:

$$v=-\frac{\kappa}{\mu}(\nabla P-\rho \mathrm{g}), \tag{3}$$

雷诺数定义为:

$$Re=\frac{\rho v d}{\mu}, \tag{4}$$

其中,v(m/s)是达西流速,κ(mD)为多孔介质渗透率,μ(Pa•s)是流体动力黏度,∇P(Pa/m)为压力梯度,ρ(kg/m^3)是流体密度,g(m/s^2)为重力常数,d

(m)是多孔介质的粒径.达西定律强调了流体的运移受到了岩石渗透率、流体压力梯度以及流体性质的影响.然而在成矿过程中因涉及气液两相流体的运移，所以达西定律可扩展为(Weis，2015)：

$$v_i = -\kappa \frac{\kappa_{ri}}{\mu_i}\left(\nabla P - \rho_i g\right),\ i = \{v, l\}, \tag{5}$$

其中，v_i是气相v或液相l的达西速度，κ_{ri}和μ_i分别为两相的相对渗透率和流体黏度.

1.3　热传递模拟

在成矿系统内热传递模拟以能量守恒为基础，依赖于传导、对流和辐射，其中主要考虑传导与对流两种方式.热传导遵循傅里叶定律：

$$Q = -kA\frac{\mathrm{d}T}{\mathrm{d}x}, \tag{6}$$

其中，Q(W)为传导的热量，k(W/(m•K))为热导率；A(m^2)为物体截面积；$\frac{\mathrm{d}T}{\mathrm{d}x}$(K/m)为温度梯度，表示温度随热传导方向距离的变化率.傅里叶定律表明，热量的传递是由高温区域向低温区域进行，同时热流的方向与温度梯度方向相反.对流所传递的热量可用牛顿冷却定律描述：

$$Q = hA(T_{\mathrm{w}} - T_{\mathrm{f}}), \tag{7}$$

其中，h(W/(m^2•K))为对流传热系数，T_{w}(K)截面温度，T_{f}(K)为流体温度.

1.4　化学反应模拟

化学反应模拟通常会基于研究的目标和问题对成矿系统内的化学反应进行简化，以计算系统内的化学平衡状态和质量平衡为约束条件，进而揭示流体性质和水岩反应的演化路径(梁祥济，1992；赵平，1992).目前，计算平衡状态主要依赖质量作用定律与系统吉布斯自由能最小化；其中，质量作用定律算法通过求解结合质量平衡与质量作用方程的非线性方程组，确定特定温度压力范围内的化学反应平衡常数K，并计算平衡状态下各物质的活度.吉布斯能最小化模型则通过限定系统中各化学元素的总量及电荷平衡来满足质量守恒，通过最小化系统内的总吉布斯自由能，以确定平衡时的物质相组合.将单个含水或气态物质或固相的吉布斯能定义为(Leal *et al.*，2017，2020)：

$$G_{i,T,P} = \Delta G^0_{i,T,P} + RT\ln a_i(\text{固相和液相}), \tag{8}$$

$$G_{i,T,P} = \Delta G^0_{i,T,P} + RT\ln f_i(\text{气相}), \tag{9}$$

其中，$\Delta G^0_{i,T,P}$(J/mol)为第i种物质的标准摩尔吉布斯自由能，a_i为固相或液相物质的活度，f_i(Pa)为气相位置的逸度.反应的标准吉布斯能的变化与反应平衡常数有关(Pokrovski，2025)：

$$\Delta_r G^0_{T,P} = \sum\nolimits_i n_i \times \Delta G^0_{i,T,P} = -2.302\,6\mathrm{R}T \times \log_{10} K_{T,P}, \tag{10}$$

其中，R是理想气体常数，为8.314 J/(mol•K)，T为开尔文温度，n_i为每种反应组分的化学计量系数，$K_{T,P}$为在给定T和P下的反应平衡常数.对于反应：

$$aA + bB = cC + dD, \tag{11}$$

$$K = \frac{C^c \times D^d}{A^a \times B^b}, \tag{12}$$

其中，A、B、C、D为反应物和产物的活度，a、b、c、d为反应中它们各自的化学计量系数，在平衡时，系统的总吉布斯能最小，即：

$$\sum G_{i,T,P} \rightarrow \min. \tag{13}$$

针对自然界许多成矿过程涉及缓慢、可逆或非均相反应，仅依靠平衡计算难以准确刻画其动态行为，所以需要通过化学动力学计算，模拟体系组成随时间的变化，从而能够提供更接近实际的瞬态描述，更好地了解化学系统的行为(於崇文，1996).针对基元反应(张有学，2010)：

$$aA + bB \rightarrow \text{生成物}, \tag{14}$$

质量作用定律将其反应速率表示为：

$$\frac{\mathrm{d}\xi}{\mathrm{d}t} = k[A]^a[B]^b, \tag{15}$$

其中，ξ(mol)为反应进度参数，k为反应速率常数，取决于具体反应和温度.其中，反应速率常数和温度的关系可应用阿伦尼乌斯方程表示：

$$k = A\exp[-E/(RT)], \tag{16}$$

其中，E(J/mol)为活化能，A为指前因子.在热液成矿研究中，基于质量作用定律的浓度梯度驱动理论将化学反应速率表述为孔隙流体流速与平衡浓度的标量积(Zhao *et al.*，2018)：

$$MR_k = v_j C^e_{k,j}, \tag{17}$$

其中，MR_k(mol/(m^2•s))为物质k的矿化率，v_j(m/s)为该方向的速度分量，C^e_k(mol/m^3)为物质k的平衡浓度.

1.5　数值计算方法

数值计算方法的核心在于将连续的求解域离散为网格单元，通过求解节点代数方程组来近似描述偏微分方程所支配的复杂系统，不同计算方法的关键区别在于其离散方法原理各异，因而在数值特性和适用范围上存在区别(李志印等，2004).

有限差分法基于经典的泰勒级数展开，直接在离散网格点上逼近偏微分方程，具有通用性强、计算方法简便和计算精度高等特点，但在处理复杂几

何边界时，其以结构化网格为基础的离散方式会带来较大拟合误差，从而影响计算精度（Thomée，2001）.有限元法的基本原理是将求解域离散为一系列具有规则几何形状且通过节点连接的单元，在每个单元内，通过选取适当的插值函数，以节点函数值的线性组合来构建该单元的近似解，从而逼近真实解.随后，采用伽辽金法等变分方法，对每个单元进行分析并建立单元方程，再将所有单元方程组合成方程组.有限元法能灵活适应复杂边界形态，并适用于多物理场耦合分析，但难以有效处理无限域问题（Ciarlet，2002；Brenner and Scott，2008）.格子玻尔兹曼法是一种基于介观模拟尺度的流体力学计算方法，具有简单的线性运算与松弛过程，兼具编程简易性与高度并行性，已然成为模拟岩石孔隙尺度下的多相多组分流体流动与传热过程的有效工具（Jiang *et al.*，2021）.

传统的数值计算方法在应对高维问题、复杂几何边界、多场耦合等科学计算难题时存在显著局限性，近年来，随着人工智能技术的快速发展，基于人工神经网络的偏微分方程求解方法作为新兴研究方向展现出突破潜力.其中，物理信息神经网络（Physics-Informed Neural Networks，PINN）通过构建逼近解的神经网络结构，在训练过程中融入物理知识，能够在数据稀疏或噪声较大的情况下仍保持良好的泛化性能，显著提升了复杂物理场建模能力（Raissi *et al.*，2019）.然而，PINN的本质是将偏微分方程求解转化为高维非凸优化问题，这也导致其常面临训练成本高昂、收敛困难且难以保证精度的局限（王飞等，2025），亟须深入研究以推动数值计算能力的跨越式提升.

2　岩浆热液矿床成矿过程研究

矿床学研究通过厘定成矿过程、建立成矿模式，为成矿预测提供核心理论依据（翟裕生，2001；李建威等，2019；陈华勇等，2022）.岩浆热液矿床的形成是由成矿物质的活化与预富集、运移与演化、沉淀与富集等一系列紧密关联的地质过程共同驱动（翟裕生，1999；Heinrich，2024）.通过对上述关键阶段中物理化学行为与动力学机制的定量模拟，不仅能够深化对成矿过程的理解，更能为定量化成矿预测提供关键约束.目前，针对岩浆热液矿床成矿过程的数值模拟主要聚焦于以下三个成岩成矿阶段：岩浆侵位与浅部岩浆房的形成、流体出溶和成矿物质的预富集、流体的运移和矿体的形成.

在第一阶段，数值模拟研究分析了地壳的地温梯度和流变强度等因素对幔源岩浆侵位过程的影响，以及岩浆房内部压力受控于岩浆补给与流体生成速率之间的平衡机制，此过程产生的热应力能在围岩中诱发大量裂隙，这些裂隙系统为后续的成矿流体提供了至关重要的运移通道与容矿空间（Huber *et al.*，2019；崔晓娜和陈林，2024；赵裕达等，2024）.深部岩浆的高速率幕式补给是形成浅部大型岩浆房、并驱动高强度大规模流体循环的关键，此类系统往往与斑岩型矿床相关，而缓慢的注入速率则倾向于形成小规模热液系统，更有利于浅成低温热液矿床的形成；同时，岩浆的初始温度、岩浆房内启动循环速率及岩浆房上边界的热传递系数对金属元素的预富集具有重要影响（Korges *et al.*，2020；Xiao *et al.*，2024a）.在第二阶段，数值模拟研究揭示了岩浆性质和冷却过程对岩浆脱气和流体出溶的时间尺度的影响，并进一步分析了这些因素对后续流体行为以及矿床规模的控制（Scott *et al.*，2017；Chelle-Michou *et al.*，2017；Gruzdeva *et al.*，2024）.同时，热力学模拟表明分离结晶作用是驱动铜从熔体中高效萃取进入流体的核心机制（Yuan *et al.*，2025）.在第三阶段，数值模拟研究主要围绕流体运移、演化、金属沉淀机制以及矿物分带特征等关键过程展开.在流体运移方面，其揭示了围岩的动态渗透率受到流体性质、热传导及岩石弹-黏-塑性的共同影响，具体表现为水力压裂通过增大围岩渗透率并引发流体压力骤降，进而通过影响金属络合物稳定性促使矿物沉淀与孔隙堵塞，最终控制了斑岩矿体的规模与空间形态（图2）（Weis *et al.*，2012，2015；Xiong *et al.*，2023）.在流体演化方面，数值模拟研究主要针对气液两相流体对金属元素的搬运能力、不同金属络合物在演化过程中的稳定性、水岩反应中流体性质的演变轨迹及矿物共生组合等方面（Zhong *et al.*，2015；Leal *et al.*，2017；Xu *et al.*，2020；杨颖等，2024；张少颖等，2024；Ma *et al.*，2025；Pokrovski，2025；Xiao *et al.*，2025）.在矿物分带特征方面，数值模拟研究表明：流体的释放速率控制了斑岩成矿系统的金属分带，矽卡岩矿床的分带模式则受到流体的氧化还原状态和由矿物沉淀引起的渗透率变化的影响（Stoltnow *et al.*，2023；常成等，2025）.此外，数值模拟方法还能够对热液矿床的单期热液矿化持续时间尺度进行限定（Zou *et al.*，

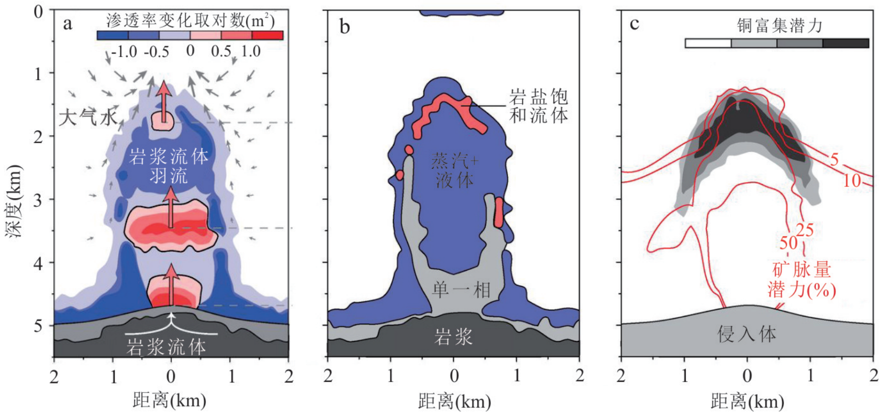

图 2　斑岩铜矿成矿过程

Fig.2　Ore-forming process of porphyry copper deposit

a、b.岩浆流体羽流及其相态；c.斑岩铜矿体富集潜力；据 Weis *et al.*(2012)

2017；Hu *et al.*，2020），研究结果与当前高精度地质年代学的新认识基本一致（Li *et al.*，2017，2023；Lin *et al.*，2024）.

综上，成矿过程数值模拟通过分析岩浆热液系统演化与金属富集的内在动力学机制，为理解矿床成因提供了定量化的理论支撑，这些基于数值模拟深化和发展的成矿理论，是构建高精度成矿预测模型、指导矿产勘查的重要理论基础.

3　控矿机理研究与成矿预测

控矿机理研究是解析岩浆热液矿床形成机制、联系成矿理论与找矿实践的重要环节.成矿过程数值模拟方法基于已有的地质数据和资料，利用定量化的分析手段，可以有针对性地分析各种地质要素对矿体空间展布特征、规模形态、品位分布等成矿特征的控制机理.在岩浆热液成矿系统中，通常情况下温度主导化学反应的动力学进程，流体运移则控制着成矿物质的输运与空间富集（Ord *et al.*，2009），因此，当前数值模拟研究主要集中于识别温度场的时空异常特征与流体的运移路径及汇聚位置，并解析其控制因素及其对成矿作用的影响.

数值模拟方法通过建立物质浓度、矿化持续时间与矿石品位之间的时空耦合关系，已经在一定程度上揭示了温度场时空异常对矿体空间展布的控制机制（图3）.研究表明，断层-褶皱构造的产状、断裂系统的空间形态、侵入体规模与产状、侵入体与围岩接触带的复杂几何形态、矿物沉淀引起的孔隙压力变化，以及不同岩石单元的物理化学性质等地质要素，主导了高温流体的瞬态演化与局部对流行为，并进一步控制了热液系统中化学反应的进程与金属沉淀的具体位置，从而影响矿体的空间分布格局，同时在揭示上述控制机制的基础上可实现对矿化潜力的定量预测（戴文强等，2019；刘向冲等，2020；Chang and Luo，2021；肖凡和王恺其，2021；Hu *et al.*，2020，2022，2023a，2023b；Gao *et al.*，2024）.

关于流体的运移和汇聚对于矿化作用的控制机制，数值模拟研究表明，热应力与流体超压驱动的岩石破碎作用会诱发局部体应变并形成扩容空间（Volumetric Strain Increment，VSI），导致成矿流体在此区域发生强烈对流并最终沉淀金属物质.当前，针对扩容空间的数值模拟研究，其核心目标在于重构成矿时的构造应力场，通过对比扩容空间和流体汇聚位置与矿体的分布规律，定量揭示“构造-流体-成矿”系统的耦合关系；在分析古应力方向、不同岩石单元力学性质、接触带形态、流体运移方向等控矿机理的基础上，采用体应变增量、最大应力、张剪应变量等力学指标指示成矿潜力（刘亮明等，2008；赵义来和刘亮明，2011；贾蔡等，2014；Gao *et al.*，2016；Zou *et al.*，2019；Shan *et al.*，2023；Mao *et al.*，2024；Xie *et al.*，2025）.

此外，在流体路径的量化表征方面，隐马尔可夫模型等随机模拟方法已被应用于重建热液系统的注入位置与运移轨迹.该类方法能够有效识别隐藏的流体通道几何形态，并提取轨迹长度与路径通量等具有成因意义的勘探指标，已在热液型金矿床研究中取得良好成效（Huang *et al.*，2024）.

综上，数值模拟方法通过定量分析成矿过程中应力、温度、流体方向等变量的演化过程及其与地质构造的耦合关系，能够有效揭示控矿机理并指示

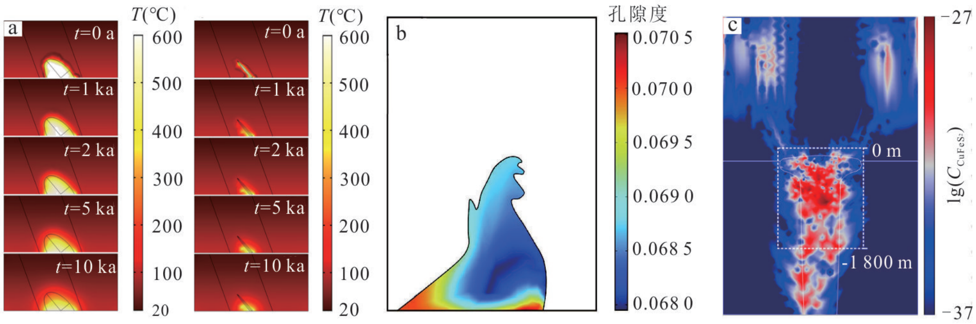

图 3　控矿机理的揭示和成矿预测

Fig.3　Analyze ore location mechanisms and facilitate metallogenic prediction

a.侵入体形态对温度场影响;b.矿石沉淀引起的渗透率变化;c.矿化潜力的预测;据肖凡和王恺其(2021)、Gao *et al.*(2024)、Hu *et al.*(2020)

成矿潜力.然而,受限于现有数值计算能力,现有研究多集中于对温度场、压力场、流体势场等物理过程的模拟,而对于水岩反应路径及最终导致矿石沉淀的关键成矿过程与其他物理场之间的动态耦合关系,相关的数值模拟目前仍有待开展更为深入的研究.

4　融合数值模拟信息的综合信息成矿预测

近年来,成矿过程数值模拟方法已成为综合信息成矿预测研究的重要数据来源.研究表明,通过运用随机森林、支持向量机等机器学习算法,可有效整合数值模拟方法获取的应力、应变、温度、流体通量、金属浓度等参数与地质、地球物理、地球化学等多元预测信息,显著提升成矿预测模型的全面性和预测能力(王语等,2020;Xiao *et al.*,2024b;肖凡和陈信宇,2025).

在深部矿产资源勘查预测领域,成矿过程数值模拟方法已成为三维成矿预测方法拓展深部预测信息的关键手段,有效缓解了传统三维成矿预测中要素缺失的瓶颈问题(图 4a)(Li *et al.*,2019;袁峰等,2019a,2024;安文通等,2021;孔维豪等,2021;毕晨曦等,2025;毛先成等,2026).机器学习模型的可解释性分析结果显示,体积应变和压力异常具有显著的特征重要性,数值模拟变量为三维成矿预测提供了重要信息支撑(Liu *et al.*,2024;Zhou and Liu,2025).

随着研究的不断深入,越来越多的数值模拟变量持续融入三维成矿预测体系.已有研究显示,三维卷积神经网络等深度学习模型可以更好地融合多元模拟变量与预测信息,有效捕捉矿化空间与预测信息间的非线性关系,提升预测结果的准确性和有效性(图 4b)(谢先岗等,2024;Zheng *et al.*,2024).此外,深度自适应网络也被认为可将浅部数值模拟揭示的成矿规律有效迁移至深部,在一定程度上增强了预测模型的泛化能力(Chen *et al.*,2024).

然而,由于岩浆热液成矿系统本质是一个多场耦合、多尺度演化的极端复杂系统,针对真实成矿过程的数值模拟研究不得不在物理化学参数与几何模型的尺度和精度上做出简化,这在一定程度上导致其对真实成矿过程的刻画能力受限,进而产生不确定性,并影响其作为预测信息的可靠性.但是可以认为,成矿过程数值模拟是从矿床学理论出发,通过揭示成矿系统的动力学过程与控矿机理输出预测信息;综合信息成矿预测方法可以与其形成互补,通过整合其他来源的预测信息在一定程度上减少数值模拟结果的不确定性对最终预测结果的影响,形成"物理机制+数据智能"的技术组合和驱动范式,不仅能将矿床学知识融入预测模型,更能显著提升成矿预测结果的有效性与可靠性.

当前,运用诸如卷积神经网络等深度学习方法的研究才刚刚起步,如何利用 Transformer 等新型架构更高效地挖掘模拟变量中的多元预测信息,是亟待探索的重要方向.此外,数值模拟所采用的网格单元尺寸通常远大于三维成矿预测单元模型的最小单元尺寸,这种尺度上的不匹配也会导致模拟结果无法承载足够精细的预测信息,最终影响三维成矿预测结果.上述问题需通过多途径解决,包括获取更精确的物理化学参数、构建更精细的几何模型、提升算力支撑等,以系统性提升综合信息成矿预测的可靠性.

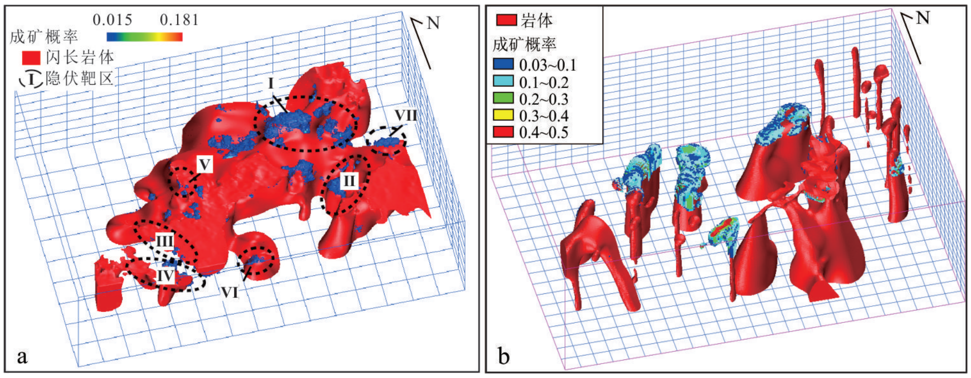

图 4　融合数值模拟信息的综合信息三维成矿预测

Fig.4　3D mineral prospectivity modeling integrating numerical modeling data

a.安庆月山地区；b.宣城狸桥地区；据 Li *et al.*（2019）、谢先岗等（2024）

5　总结与展望

成矿过程数值模拟在刻画岩浆热液矿床的成矿过程、揭示控矿机理以及融合数值模拟信息的成矿预测等方面取得了大量研究成果，已成为深化岩浆热液矿床成因认识和指导成矿预测的关键工具．然而，随着找矿勘查工作向深部、隐伏矿体等复杂场景推进，数值模拟和成矿预测方法仍面临一系列亟待突破的挑战，同时也在新技术的驱动下展现出广阔的发展前景．

（1）未来研究将致力于发展力-热-化-流全耦合数值模拟，重点关注流体性质演化和矿物沉淀机制与流体动力学的耦合关系．同时，也需进一步探索如何更真实地还原成矿时的物理化学环境，获取更合理的初始边界条件与岩石物性参数，以提升模型的地质可信度与预测能力．

（2）在数值计算方法方面，传统有限元、有限差分等手段在处理复杂地质模型与多物理场耦合问题时，时常面临高维非线性带来的计算效率与精度瓶颈．未来应着力发展适应复杂地质结构的高性能数值技术，以更有效地表征真实成矿条件，从而获取更为可靠的成矿过程信息与找矿指示标志．

（3）融合成矿过程数值模拟信息的三维成矿预测是未来重要的研究方向．其关键在于挖掘更多成矿过程数值模拟信息要素，突破数据融合与模型构建中的技术瓶颈，发展多尺度、多机制融合的智能预测新方法，从而推动成矿预测向“物理机制＋数据智能”驱动范式转变．

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